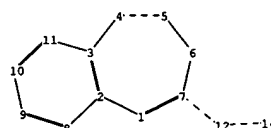
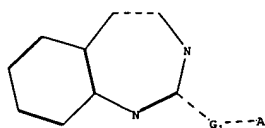


10019683



ring nodes :

1 2 3 4 5 6 7 8 9 10 11

ring/chain nodes :

12 14

ring/chain bonds :

7-12 12-14

ring bonds :

1-2 1-7 2-3 2-8 3-4 3-11 4-5 5-6 6-7 8-9 9-10 10-11

exact/norm bonds :

1-2 1-7 3-4 4-5 5-6 6-7 7-12 12-14

normalized bonds :

2-3 2-8 3-11 8-9 9-10 10-11

G1:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS
14:CLASS

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=> d his

(FILE 'HOME' ENTERED AT 16:27:24 ON 29 AUG 2006)

FILE 'REGISTRY' ENTERED AT 16:27:34 ON 29 AUG 2006

L1 STRUCTURE UPLOADED

L2 11 S L1

L3 STRUCTURE UPLOADED

L4 3 S L3

L5 2192 S L1 SSS FUL

L6 775 S L3 SUB=L5 FUL

FILE 'CAPLUS' ENTERED AT 16:37:14 ON 29 AUG 2006

L7 56 S L6

L8 53 S L7 NOT (2006/SO OR 2005/SO OR 2004/SO OR 2003/SO OR 2002/SO O

FILE 'REGISTRY' ENTERED AT 16:38:45 ON 29 AUG 2006

L9 STRUCTURE UPLOADED

L10 3 S L9

L11 800 S L9 SSS FUL

FILE 'CAPLUS' ENTERED AT 16:39:21 ON 29 AUG 2006

L12 59 S L11

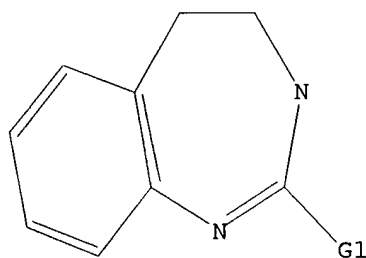
L13 3 S L7 NOT L8

L14 56 S L12 NOT L13

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 O,S,N

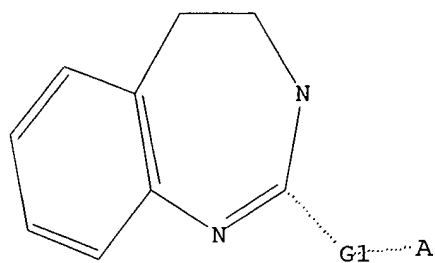
Structure attributes must be viewed using STN Express query preparation.

=> d l3

L3 HAS NO ANSWERS

L3 STR

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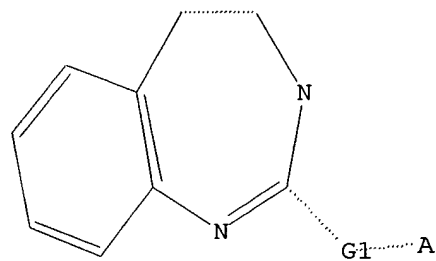
G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> d 19

L9 HAS NO ANSWERS

L9 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> d ibib abs hitstr total 114

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514 ANSWER 1 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:358147 CAPLUS

Correction of: 2005:481369

DOCUMENT NUMBER: 145:123919

Correction of: 143:26019

TITLE: Carbon dioxide, carbonyl sulfide, carbon disulfide, isocyanates, isothiocyanates, carbodiimides, and their selenium, tellurium, and phosphorus analogues

AUTHOR(S): Braverman, S.; Cherkinsky, M.; Birsa, M. L.

CORPORATE SOURCE: Dept. of Chemistry, Bar-Ilan University, Ramat-Gan, 52900, Israel

SOURCE: Science of Synthesis (2005), 18, 65-320

CODEN: SSCYJ9

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review of the application of carbon dioxide, carbonyl sulfide, carbon disulfide, isocyanates, isothiocyanates, carbodiimides, and their selenium, tellurium, and phosphorus analog to organic synthesis.

IT 199390-42-6P 199390-43-7P 199390-45-9P

199390-46-0P 199390-47-1P 199390-48-2P

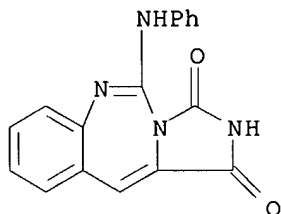
199390-49-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthetic applications of carbon dioxide, carbonyl sulfide, carbon disulfide, isocyanates, isothiocyanates, carbodiimides, and their selenium, tellurium, and phosphorus analogs)

RN 199390-42-6 CAPLUS

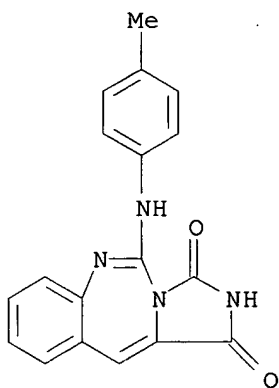
CN 1H-Imidazo[1,5-c][1,3]benzodiazepine-1,3(2H)-dione, 5-(phenylamino)- (9CI)
(CA INDEX NAME)



RN 199390-43-7 CAPLUS

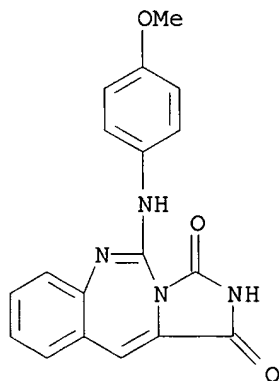
CN 1H-Imidazo[1,5-c][1,3]benzodiazepine-1,3(2H)-dione, 5-[(4-methylphenyl)amino]- (9CI) (CA INDEX NAME)

10/019,683



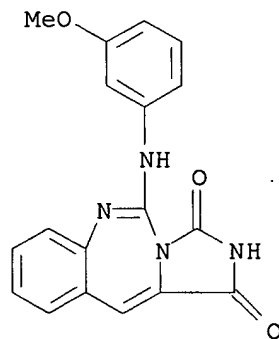
RN 199390-45-9 CAPLUS

CN 1H-Imidazo[1,5-c][1,3]benzodiazepine-1,3(2H)-dione, 5-[(4-methoxyphenyl)amino]- (9CI) (CA INDEX NAME)



RN 199390-46-0 CAPLUS

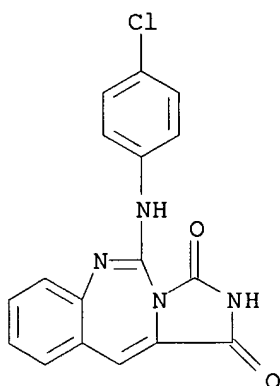
CN 1H-Imidazo[1,5-c][1,3]benzodiazepine-1,3(2H)-dione, 5-[(3-methoxyphenyl)amino]- (9CI) (CA INDEX NAME)



RN 199390-47-1 CAPLUS

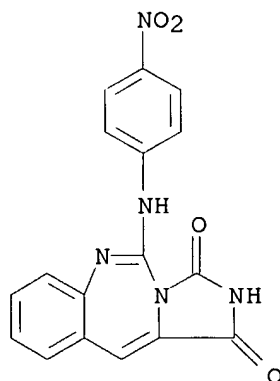
10/019,683

CN 1H-Imidazo[1,5-c][1,3]benzodiazepine-1,3(2H)-dione, 5-[(4-chlorophenyl)amino]- (9CI) (CA INDEX NAME)



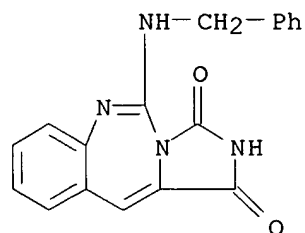
RN 199390-48-2 CAPLUS

CN 1H-Imidazo[1,5-c][1,3]benzodiazepine-1,3(2H)-dione, 5-[(4-nitrophenyl)amino]- (9CI) (CA INDEX NAME)



RN 199390-49-3 CAPLUS

CN 1H-Imidazo[1,5-c][1,3]benzodiazepine-1,3(2H)-dione, 5-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



~~IN4~~ ANSWER 2 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

~~AC~~CESSION NUMBER: 2006:100738 CAPLUS

DOCUMENT NUMBER: 144:198849

TITLE: Novel dosage form comprising modified-release and immediate-release active ingredients

INVENTOR(S): Vaya, Navin; Karan, Rajesh Singh; Sadanand, Sunil; Gupta, Vinod Kumar

PATENT ASSIGNEE(S): India

SOURCE: U.S. Pat. Appl. Publ., 49 pp., Cont.-in-part of U.S. Ser. No. 630,446.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| US 2006024365 | A1 | 20060202 | US 2005-134633 | 20050519 |
| IN 193042 | A | 20040626 | IN 2002-MU697 | 20020805 |
| US 2004096499 | A1 | 20040520 | US 2003-630446 | 20030729 |
| PRIORITY APPLN. INFO.: | | | IN 2002-MU697 | A 20020805 |
| | | | IN 2002-MU699 | A 20020805 |
| | | | IN 2003-MU80 | A 20030122 |
| | | | IN 2003-MU82 | A 20030122 |
| | | | US 2003-630446 | A2 20030729 |

AB A dosage form comprising of a high dose, high solubility active ingredient as modified release and a low dose active ingredient as immediate release where the weight ratio of immediate release active ingredient and modified release active ingredient is from 1:10 to 1:15000 and the weight of modified release active ingredient per unit is from 500 mg to 1500 mg; a process for preparing the dosage form. Tablets containing 10 mg sodium pravastatin and 1000 mg niacin were prepared. The release of sodium pravastatin after 24 h was 67.7%, and the release of niacin after 1 h was 84.1%.

IT 120360-10-3, Batelapine maleate

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel dosage form comprising modified-release and immediate-release active ingredients)

RN 120360-10-3 CAPLUS

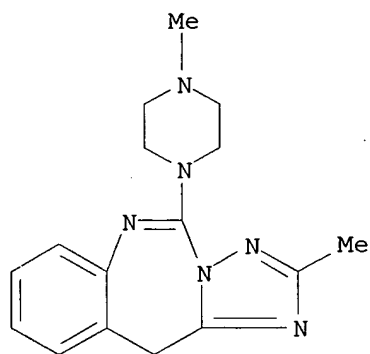
CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 2-methyl-5-(4-methyl-1-piperazinyl)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 95634-82-5

CMF C16 H20 N6

10/019,683

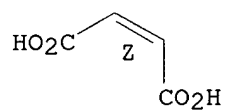


CM 2

CRN 110-16-7

CMF C4 H4 O4

Double bond geometry as shown.



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~~LA~~ ANSWER 3 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:837076 CAPLUS

DOCUMENT NUMBER: 139:337970

TITLE: Preparation of piperidine derivatives as CCR3 antagonists

INVENTOR(S): Matsumoto, Yoshiyuki; Imai, Minoru; Sawai, Yoshiyuki; Takeuchi, Susumu; Nakanishi, Akinobu; Minamizono, Kunio; Yokoyama, Tomonori

PATENT ASSIGNEE(S): Teijin Limited, Japan

SOURCE: PCT Int. Appl., 564 pp.

CODEN: PIXXD2

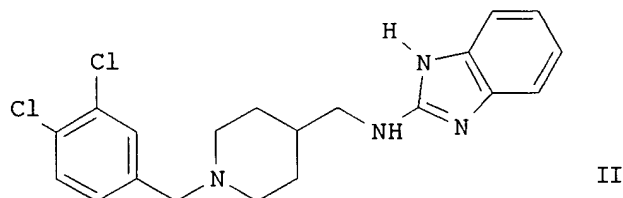
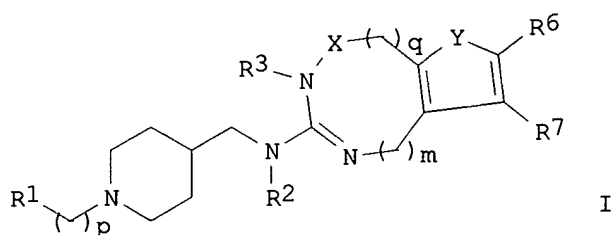
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|-------------------|----------|-----------------|------------|
| WO 2003087089 | A1 | 20031023 | WO 2003-JP4841 | 20030416 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2484261 | AA | 20031023 | CA 2003-2484261 | 20030416 |
| AU 2003231359 | A1 | 20031027 | AU 2003-231359 | 20030416 |
| EP 1502916 | A1 | 20050202 | EP 2003-725592 | 20030416 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| CN 1659161 | A | 20050824 | CN 2003-813754 | 20030416 |
| PRIORITY APPLN. INFO.: | | | JP 2002-113220 | A 20020416 |
| | | | JP 2002-240509 | A 20020821 |
| | | | WO 2003-JP4841 | W 20030416 |
| OTHER SOURCE(S): | MARPAT 139:337970 | | | |
| GI | | | | |



AB The title piperidine derivs. having a benzimidazole subunit with general formula of I [wherein R1 = cycloalkyl, aromatic heterocyclyl, or (un)substituted Ph, etc.; p = 0-6; R2 and R3 = independently H, (un)substituted alkyl, or Ph; X = CO, SO2, CH2, CS, or a single bond; q = 0 or 1; m = 0 or 1; Y = S, -CR4=CR5-, or (un)substituted -NH-; R4-R7 = independently H, halo, OH, CN, NO2, CO2H, alkyl, cycloalkyl, alkenyl, alkoxy, alkylthio, alkylene, alkyleneoxy, alkylenedioxy, Ph, PhO, PhS, PhSO2, PhCH2, PhCH2O, PhCONH, CHO, alkanoyl(oxy), alkoxy-CO, (cyclo)alkanoylamino, alkenoylamino, alkyl-SO2, alkyl-SO2NH, alkoxy-CO-CH2, pyridyl-CO, morpholyl-CO, pyrrolidinyl-CO, piperazinyl-CO, ureido, thioureido, (un)substituted NH2, carbamoyl, or SO2NH, etc.] and pharmaceutically acceptable salts, or alkyl adducts thereof are prepared as chemokine receptor 3 (CCR3) antagonists. For example, the compound II was prepared in a multi-step synthesis. Some of compds. I showed >80% inhibitory activity at the concentration of 2 μ M against CCR3. I are useful for the treatment of diseases in which CCR3 participates such as asthma and allergic nephritis, etc. (no data).

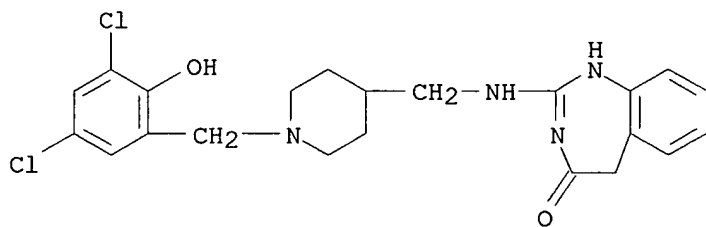
IT 616223-92-8P 616223-93-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of piperidine derivs. as CCR3 antagonists)

RN 616223-92-8 CAPLUS

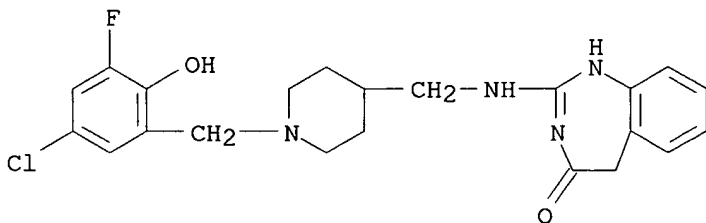
CN 4H-1,3-Benzodiazepin-4-one, 2-[[[1-[(3,5-dichloro-2-hydroxyphenyl)methyl]-4-piperidinyl)methyl]amino]-1,5-dihydro- (9CI) (CA INDEX NAME)



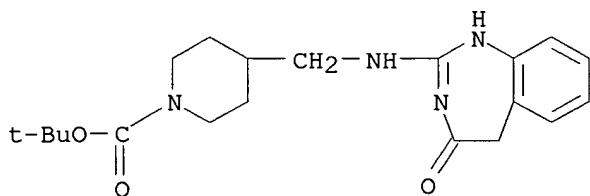
RN 616223-93-9 CAPLUS

10/019,683

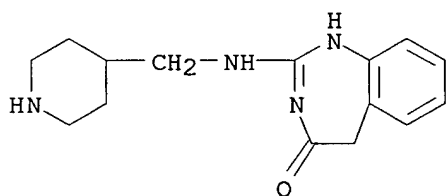
CN 4H-1,3-Benzodiazepin-4-one, 2-[[[1-[(5-chloro-3-fluoro-2-hydroxyphenyl)methyl]-4-piperidinyl)methyl]amino]-1,5-dihydro- (9CI) (CA INDEX NAME)



IT 616225-01-5P 616225-02-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of piperidine derivs. as CCR3 antagonists)
RN 616225-01-5 CAPLUS
CN 1-Piperidinecarboxylic acid, 4-[[[4,5-dihydro-4-oxo-1H-1,3-benzodiazepin-2-yl)amino]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 616225-02-6 CAPLUS
CN 4H-1,3-Benzodiazepin-4-one, 1,5-dihydro-2-[(4-piperidinylmethyl)amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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114 ANSWER 4 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:777651 CAPLUS

DOCUMENT NUMBER: 137:294988

TITLE: Cyanamide, alkoxyamino, and urea derivatives of
1,3-benzodiazapines as HIV reverse transcriptase
inhibitors

INVENTOR(S): Bilder, Donna M.

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 117 pp.

CODEN: PIXXD2

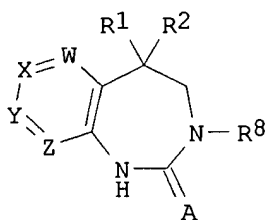
DOCUMENT TYPE: Patent

LANGUAGE: English

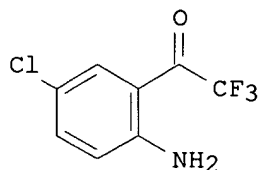
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

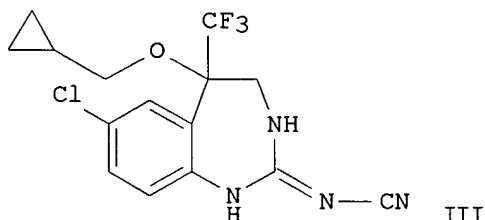
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--|----------|-----------------|------------|
| WO 2002078628 | A2 | 20021010 | WO 2002-US9456 | 20020327 |
| WO 2002078628 | A3 | 20030327 | | |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW | | | |
| RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
| US 2003220327 | A1 | 20031127 | US 2002-108842 | 20020327 |
| US 7015214 | B2 | 20060321 | | |
| PRIORITY APPLN. INFO.: | | | US 2001-279217P | P 20010328 |
| OTHER SOURCE(S): | MARPAT 137:294988 | | | |
| GI | | | | |



I



II



III

AB Title compds. I [A = NCN, NCONH, N-alkoxy; W = N, CR₃; X = N, CR_{3a}; Y = N, CR_{3b}; Z = N, CR_{3c}; provided that if two of W, X, Y, and Z are N, then the remaining are other than N; R₁ = alkyl; R₂ = R_{2c}, OR_{2c}, etc.; R_{2c} = alk(en/yn)yl, cycloalkyl, Ph, etc.; R₃ = H, alkyl, OH, alkoxy, OCF₃, etc.; R_{3a} = H, alkyl, OH, alkoxy, OCF₃, F, Cl, Br, etc.; R_{3b} = H, alkyl, OH, alkoxy, OCF₃, F, Cl, Br, etc.; R_{3c} = H, alkyl, OH, alkoxy, OCF₃, F, Cl, Br, etc.; R₈ = H, alkoxy, thioalkoxy, amino, alkyl, etc.] were prepared For instance, II was subjected to the following sequence: i. DMSO/THF, Me₃SOI, NaH; ii. EtOH, NH₃, 45°, 2 days; iii. IPA, diphenylcyanocarbonimide; iv. DMSO, NaH, BrCH₂Pr-c to afford III. I are useful as inhibitors of HIV reverse transcriptase, and to pharmaceutical compns. and diagnostic kits comprising the same, and methods of using the same for treating viral infection or as an assay standard or reagent.

IT 467240-84-2P 467240-94-4P 467240-96-6P,
7-Chloro-2-cyanoimino-5-(cyclopropylmethoxy)-1,5-dihydro-3-ethyl-5-trifluoromethyl-1,3-benzodiazepine 467241-02-7P
467241-12-9P, 7-Chloro-5-cyclopropylmethoxy-1,5-dihydro-3-ethyl-2-methoxyimino-5-trifluoromethyl-1,3-benzodiazepine 467241-13-0P
467241-14-1P 467241-15-2P 467241-16-3P
467241-17-4P 467241-18-5P 467241-19-6P
467241-20-9P 467241-21-0P 467241-22-1P

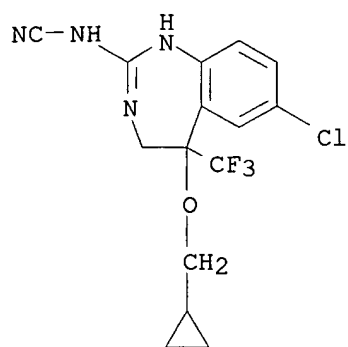
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(HIV reverse transcriptase inhibitor; cyanamide, alkoxyamino, and urea derivs. of 1,3-benzodiazepines as HIV reverse transcriptase inhibitors)

RN 467240-84-2 CAPLUS

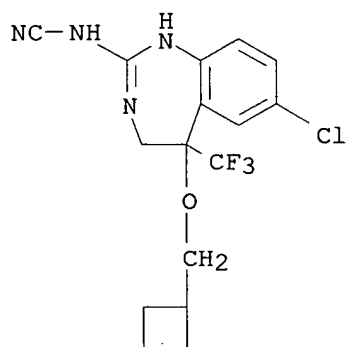
CN Cyanamide, [7-chloro-5-(cyclopropylmethoxy)-4,5-dihydro-5-(trifluoromethyl)-1H-1,3-benzodiazepin-2-yl]- (9CI) (CA INDEX NAME)

10/019,683



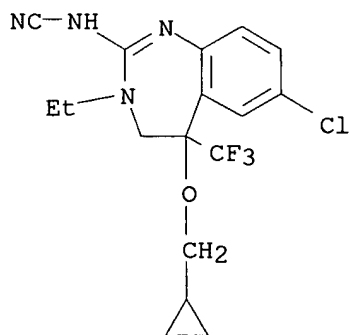
RN 467240-94-4 CAPLUS

CN Cyanamide, [7-chloro-5-(cyclobutylmethoxy)-4,5-dihydro-5-(trifluoromethyl)-1H-1,3-benzodiazepin-2-yl]- (9CI) (CA INDEX NAME)



RN 467240-96-6 CAPLUS

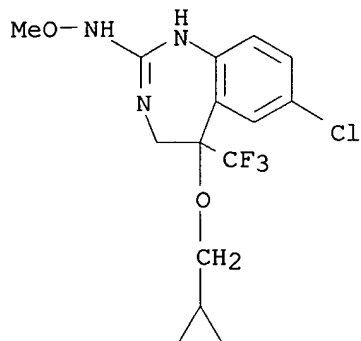
CN Cyanamide, [7-chloro-5-(cyclopropylmethoxy)-3-ethyl-4,5-dihydro-5-(trifluoromethyl)-3H-1,3-benzodiazepin-2-yl]- (9CI) (CA INDEX NAME)



RN 467241-02-7 CAPLUS

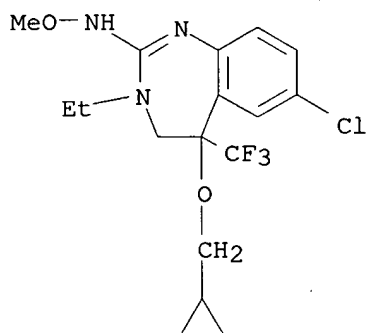
CN 2H-1,3-Benzodiazepin-2-one, 7-chloro-5-(cyclopropylmethoxy)-1,3,4,5-tetrahydro-5-(trifluoromethyl)-, O-methyloxime (9CI) (CA INDEX NAME)

10/019,683



RN 467241-12-9 CAPLUS

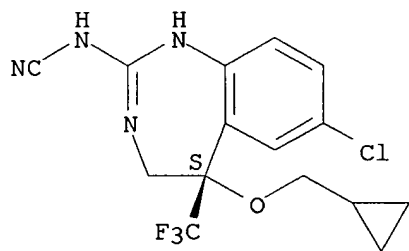
CN 2H-1,3-Benzodiazepin-2-one, 7-chloro-5-(cyclopropylmethoxy)-3-ethyl-1,3,4,5-tetrahydro-5-(trifluoromethyl)-, O-methyloxime (9CI) (CA INDEX NAME)



RN 467241-13-0 CAPLUS

CN Cyanamide, [(5S)-7-chloro-5-(cyclopropylmethoxy)-4,5-dihydro-5-(trifluoromethyl)-1H-1,3-benzodiazepin-2-yl]- (9CI) (CA INDEX NAME)

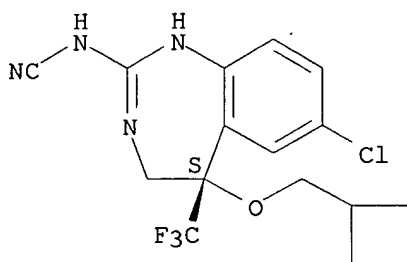
Absolute stereochemistry.



RN 467241-14-1 CAPLUS

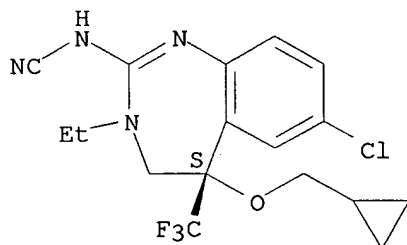
CN Cyanamide, [(5S)-7-chloro-5-(cyclobutylmethoxy)-4,5-dihydro-5-(trifluoromethyl)-1H-1,3-benzodiazepin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



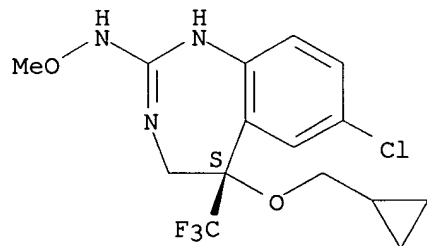
RN 467241-15-2 CAPLUS
 CN Cyanamide, [7-chloro-5-(cyclopropylmethoxy)-3-ethyl-4,5-dihydro-5-(trifluoromethyl)-3H-1,3-benzodiazepin-2-yl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



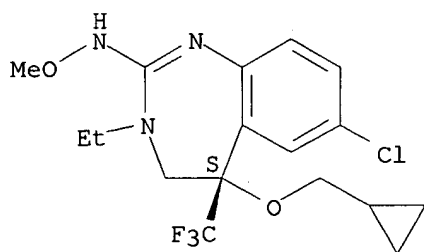
RN 467241-16-3 CAPLUS
 CN 2H-1,3-Benzodiazepin-2-one, 7-chloro-5-(cyclopropylmethoxy)-1,3,4,5-tetrahydro-5-(trifluoromethyl)-, O-methyloxime, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 467241-17-4 CAPLUS
 CN 2H-1,3-Benzodiazepin-2-one, 7-chloro-5-(cyclopropylmethoxy)-3-ethyl-1,3,4,5-tetrahydro-5-(trifluoromethyl)-, O-methyloxime, (5S)- (9CI) (CA INDEX NAME)

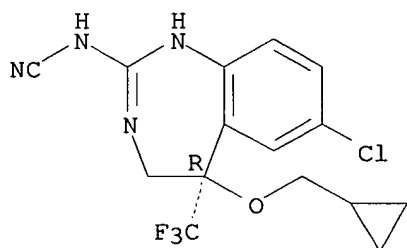
Absolute stereochemistry.



RN 467241-18-5 CAPLUS

CN Cyanamide, [(5R)-7-chloro-5-(cyclopropylmethoxy)-4,5-dihydro-5-(trifluoromethyl)-1H-1,3-benzodiazepin-2-yl]- (9CI) (CA INDEX NAME)

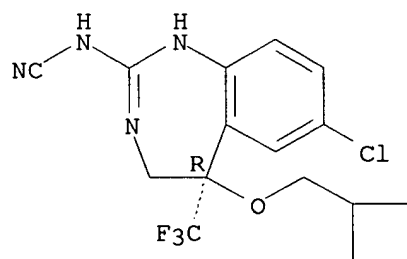
Absolute stereochemistry.



RN 467241-19-6 CAPLUS

CN Cyanamide, [(5R)-7-chloro-5-(cyclobutylmethoxy)-4,5-dihydro-5-(trifluoromethyl)-1H-1,3-benzodiazepin-2-yl]- (9CI) (CA INDEX NAME)

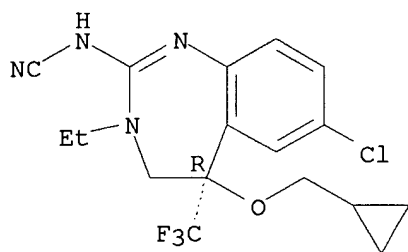
Absolute stereochemistry.



RN 467241-20-9 CAPLUS

CN Cyanamide, [7-chloro-5-(cyclopropylmethoxy)-3-ethyl-4,5-dihydro-5-(trifluoromethyl)-3H-1,3-benzodiazepin-2-yl]-, (5R)- (9CI) (CA INDEX NAME)

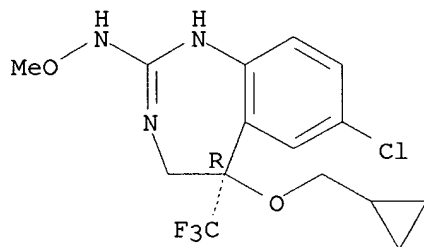
Absolute stereochemistry.



RN 467241-21-0 CAPLUS

CN 2H-1,3-Benzodiazepin-2-one, 7-chloro-5-(cyclopropylmethoxy)-1,3,4,5-tetrahydro-5-(trifluoromethyl)-, O-methyloxime, (5R)- (9CI) (CA INDEX NAME)

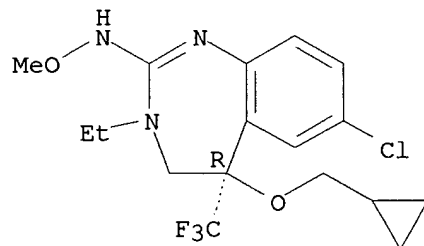
Absolute stereochemistry.



RN 467241-22-1 CAPLUS

CN 2H-1,3-Benzodiazepin-2-one, 7-chloro-5-(cyclopropylmethoxy)-3-ethyl-1,3,4,5-tetrahydro-5-(trifluoromethyl)-, O-methyloxime, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 467240-92-2P 467241-11-8P

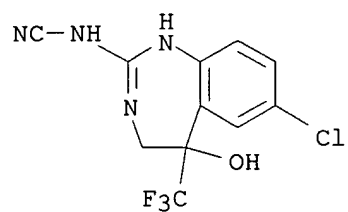
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; cyanamide, alkoxyamino, and urea derivs. of 1,3-benzodiazepines as HIV reverse transcriptase inhibitors)

RN 467240-92-2 CAPLUS

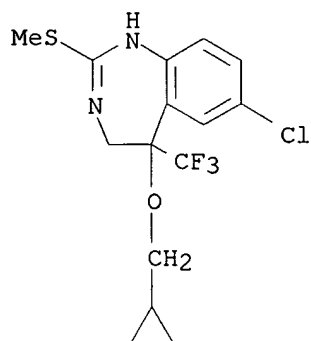
CN Cyanamide, [7-chloro-4,5-dihydro-5-hydroxy-5-(trifluoromethyl)-1H-1,3-benzodiazepin-2-yl]- (9CI) (CA INDEX NAME)

10/019,683



RN 467241-11-8 CAPLUS

CN 1H-1,3-Benzodiazepine, 7-chloro-5-(cyclopropylmethoxy)-4,5-dihydro-2-(methylthio)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



10/019,683

L14 ANSWER 5 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:31477 CAPLUS

DOCUMENT NUMBER: 134:100893

TITLE: Preparation of dihydrobenzodiazepines and their use for treating dyslipidemia

INVENTOR(S): Berthelon, Jean-Jacques; Guerrier, Daniel; Brunet, Michel; Zeiller, Jean-Jacques; Contard, Francis; Ausseil, Frederic

PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany

SOURCE: PCT Int. Appl., 101 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: French

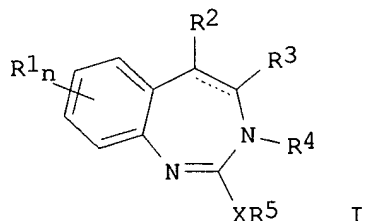
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 2001002373 | A1 | 20010111 | WO 2000-EP6230 | 20000704 |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, MD | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| FR 2796070 | A1 | 20010112 | FR 1999-8714 | 19990706 |
| FR 2796070 | B1 | 20030221 | | |
| CA 2378165 | AA | 20010111 | CA 2000-2378165 | 20000704 |
| BR 2000012169 | A | 20020319 | BR 2000-12169 | 20000704 |
| EP 1189890 | A1 | 20020327 | EP 2000-945864 | 20000704 |
| EP 1189890 | B1 | 20060419 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY | | | | |
| JP 2003503483 | T2 | 20030128 | JP 2001-507812 | 20000704 |
| AU 767016 | B2 | 20031030 | AU 2000-59814 | 20000704 |
| RU 2247115 | C2 | 20050227 | RU 2002-102248 | 20000704 |
| AT 323685 | E | 20060515 | AT 2000-945864 | 20000704 |
| NO 2002000031 | A | 20020305 | NO 2002-31 | 20020104 |
| ZA 2002001008 | A | 20030609 | ZA 2002-1008 | 20020205 |
| PRIORITY APPLN. INFO.: | | | FR 1999-8714 | A 19990706 |
| | | | WO 2000-EP6230 | W 20000704 |

OTHER SOURCE(S): MARPAT 134:100893

GI



AB Benzodiazepines I [R1 = alkyl, alkoxy, halo, NO2, etc.; n = 0-4; R2, R3 =

H, alkyl, aryl, heteroaryl, etc.; R4 = H, alkyl, aryl, OH, etc.; X = S, O, NT and T = H, alkyl, aryl, etc.; R5 = alkyl, hydroxyalkyl, arylalkyl, etc.], useful for treating dyslipidemia, were prepared E.g.,
 3-(biphenyl-3-yl)-5,6-dihydrothiazolo[2,3-b]-1,3-benzodiazepine was prepared

IT 318529-44-1P 318529-45-2P 318529-46-3P
 318529-47-4P 318529-48-5P 318529-49-6P
 318529-50-9P 318529-51-0P 318529-52-1P
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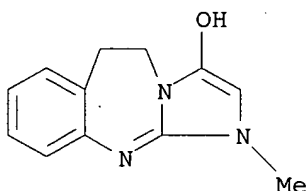
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 318531-33-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of dihydrobenzodiazepines and their use for treating dyslipidemia)

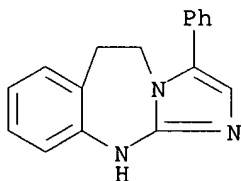
RN 318529-44-1 CAPLUS

CN 1H-Imidazo[2,1-b][1,3]benzodiazepin-3-ol, 5,6-dihydro-1-methyl- (9CI) (CA INDEX NAME)



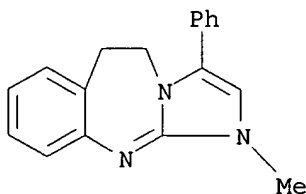
RN 318529-45-2 CAPLUS

CN 1H-Imidazo[2,1-b][1,3]benzodiazepine, 5,6-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



RN 318529-46-3 CAPLUS

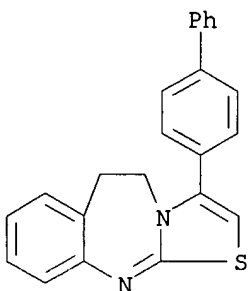
CN 1H-Imidazo[2,1-b][1,3]benzodiazepine, 5,6-dihydro-1-methyl-3-phenyl- (9CI) (CA INDEX NAME)



RN 318529-47-4 CAPLUS

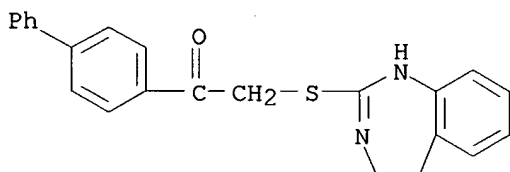
10/019,683

CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-[1,1'-biphenyl]-4-yl-5,6-dihydro-
(9CI) (CA INDEX NAME)



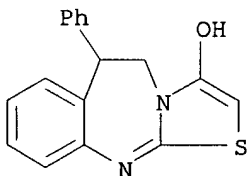
RN 318529-48-5 CAPLUS

CN Ethanone, 1-[1,1'-biphenyl]-4-yl-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



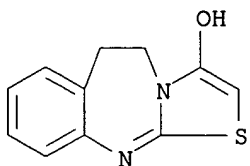
RN 318529-49-6 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepin-3-ol, 5,6-dihydro-6-phenyl- (9CI) (CA INDEX NAME)



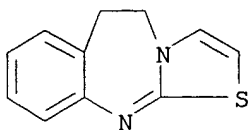
RN 318529-50-9 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepin-3-ol, 5,6-dihydro- (9CI) (CA INDEX NAME)

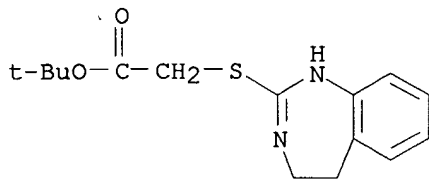


RN 318529-51-0 CAPLUS

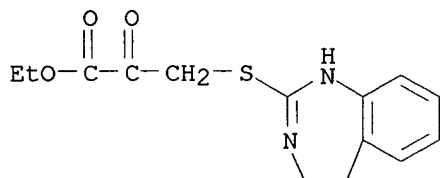
CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro- (9CI) (CA INDEX NAME)



RN 318529-52-1 CAPLUS
 CN Acetic acid, [(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

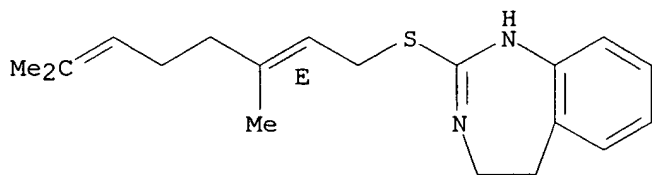


RN 318529-53-2 CAPLUS
 CN Propanoic acid, 3-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 318529-54-3 CAPLUS
 CN 1H-1,3-Benzodiazepine, 2-[[(2E)-3,7-dimethyl-2,6-octadienyl]thio]-4,5-dihydro-, monohydrobromide (9CI) (CA INDEX NAME)

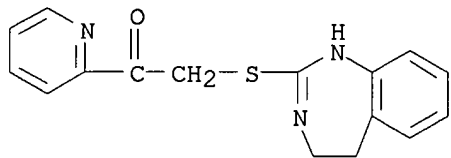
Double bond geometry as shown.



● HBr

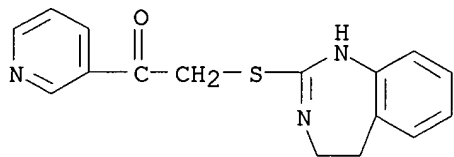
RN 318529-55-4 CAPLUS
 CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(2-pyridinyl)- (9CI) (CA INDEX NAME)

10/019,683



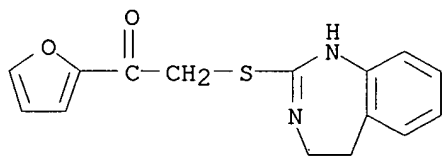
RN 318529-56-5 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(3-pyridinyl)-
(9CI) (CA INDEX NAME)



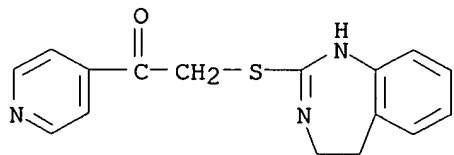
RN 318529-57-6 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(2-furanyl)-
(9CI) (CA INDEX NAME)



RN 318529-58-7 CAPLUS

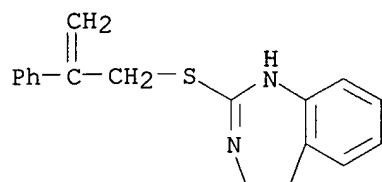
CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(4-pyridinyl)-
(9CI) (CA INDEX NAME)



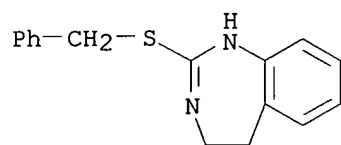
RN 318529-59-8 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-[(2-phenyl-2-propenyl)thio]- (9CI)
(CA INDEX NAME)

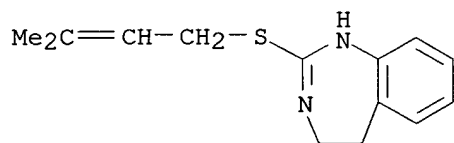
10/019,683



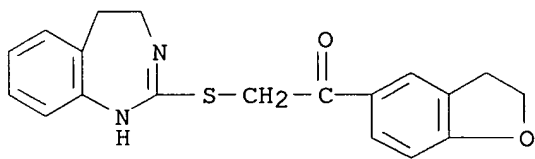
RN 318529-60-1 CAPLUS
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)



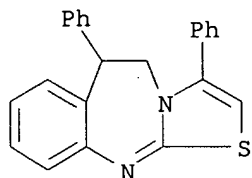
RN 318529-61-2 CAPLUS
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-[(3-methyl-2-butenyl)thio]- (9CI) (CA INDEX NAME)



RN 318529-62-3 CAPLUS
CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(2,3-dihydro-5-benzofuranyl)- (9CI) (CA INDEX NAME)

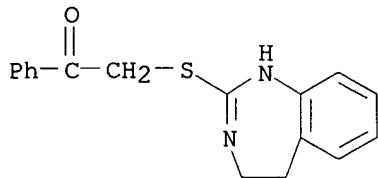


RN 318529-63-4 CAPLUS
CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3,6-diphenyl- (9CI) (CA INDEX NAME)



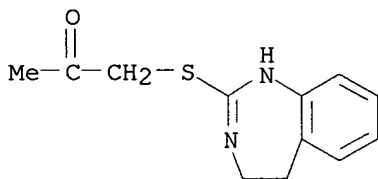
RN 318529-64-5 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-phenyl- (9CI)
(CA INDEX NAME)



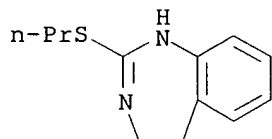
RN 318529-65-6 CAPLUS

CN 2-Propanone, 1-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



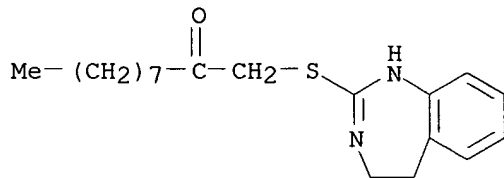
RN 318529-66-7 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(propylthio)- (9CI) (CA INDEX NAME)



RN 318529-67-8 CAPLUS

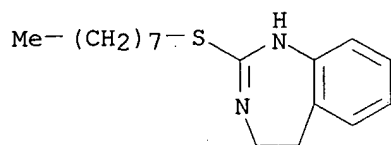
CN 2-Decanone, 1-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



RN 318529-68-9 CAPLUS

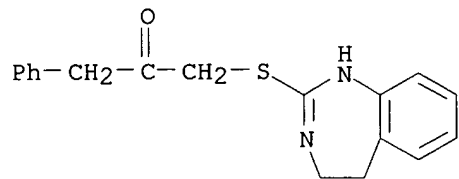
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(octylthio)- (9CI) (CA INDEX NAME)

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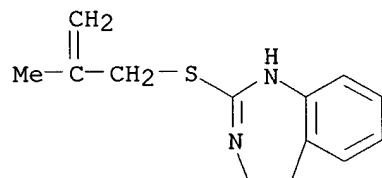
RN 318529-69-0 CAPLUS

CN 2-Propanone, 1-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-3-phenyl-
(9CI) (CA INDEX NAME)



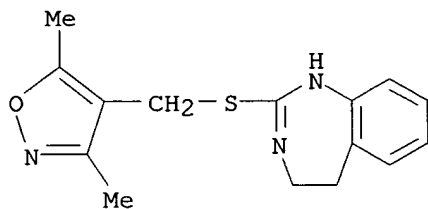
RN 318529-70-3 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-[(2-methyl-2-propenyl)thio]- (9CI)
(CA INDEX NAME)



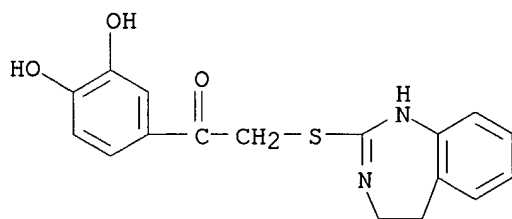
RN 318529-71-4 CAPLUS

CN 1H-1,3-Benzodiazepine, 2-[[[(3,5-dimethyl-4-isoxazolyl)methyl]thio]-4,5-
dihydro- (9CI) (CA INDEX NAME)

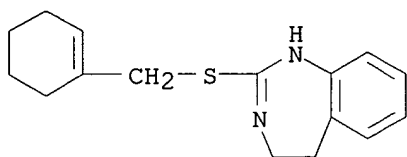


RN 318529-72-5 CAPLUS

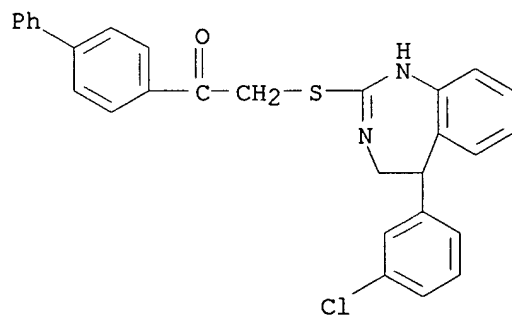
CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(3,4-
dihydroxyphenyl)- (9CI) (CA INDEX NAME)



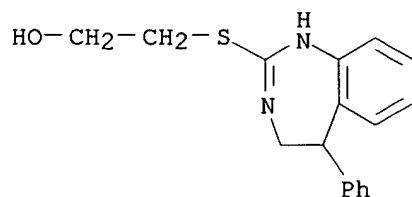
RN 318529-73-6 CAPLUS
CN 1H-1,3-Benzodiazepine, 2-[(1-cyclohexen-1-ylmethyl)thio]-4,5-dihydro-
(9CI) (CA INDEX NAME)



RN 318529-74-7 CAPLUS
CN Ethanone, 1-[1,1'-biphenyl]-4-yl-2-[[5-(3-chlorophenyl)-4,5-dihydro-1H-1,3-benzodiazepin-2-yl]thio]- (9CI) (CA INDEX NAME)



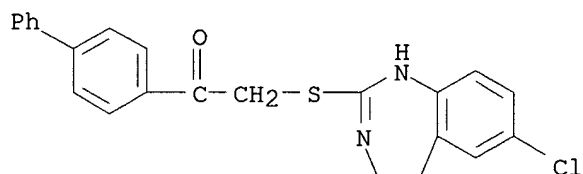
RN 318529-75-8 CAPLUS
CN Ethanol, 2-[(4,5-dihydro-5-phenyl-1H-1,3-benzodiazepin-2-yl)thio]- (9CI)
(CA INDEX NAME)



RN 318529-76-9 CAPLUS
CN Ethanone, 1-[1,1'-biphenyl]-4-yl-2-[(7-chloro-4,5-dihydro-1H-1,3-

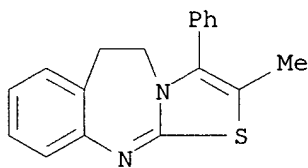
10/019,683

benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



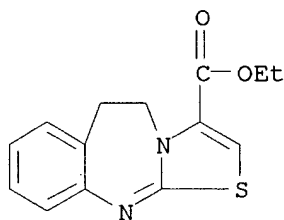
RN 318529-77-0 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-2-methyl-3-phenyl- (9CI)
(CA INDEX NAME)



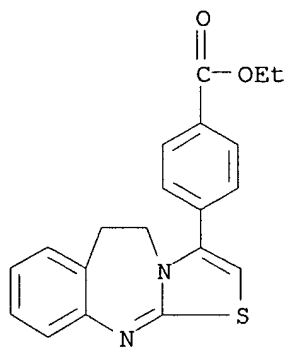
RN 318529-78-1 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine-3-carboxylic acid, 5,6-dihydro-, ethyl
ester (9CI) (CA INDEX NAME)



RN 318529-79-2 CAPLUS

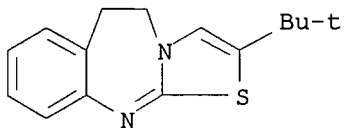
CN Benzoic acid, 4-(5,6-dihydrothiazolo[2,3-b][1,3]benzodiazepin-3-yl)-,
ethyl ester (9CI) (CA INDEX NAME)



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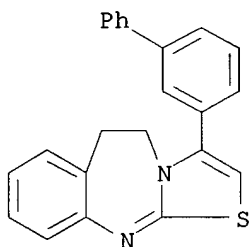
RN 318529-80-5 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 2-(1,1-dimethylethyl)-5,6-dihydro-
(9CI) (CA INDEX NAME)



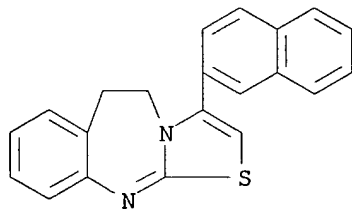
RN 318529-81-6 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-[1,1'-biphenyl]-3-yl-5,6-dihydro-
(9CI) (CA INDEX NAME)



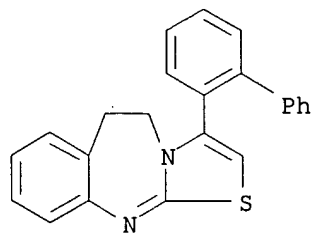
RN 318529-82-7 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(2-naphthalenyl)- (9CI)
(CA INDEX NAME)



RN 318529-83-8 CAPLUS

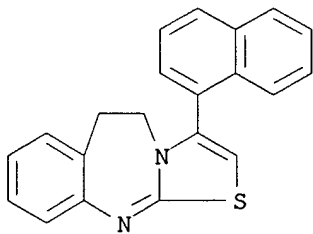
CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-[1,1'-biphenyl]-2-yl-5,6-dihydro-
(9CI) (CA INDEX NAME)



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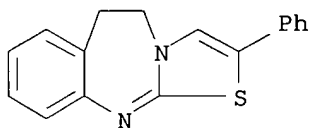
RN 318529-84-9 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(1-naphthalenyl)- (9CI)
(CA INDEX NAME)



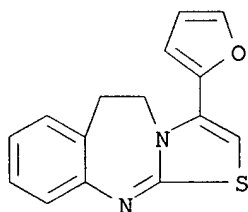
RN 318529-85-0 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-2-phenyl- (9CI) (CA INDEX NAME)



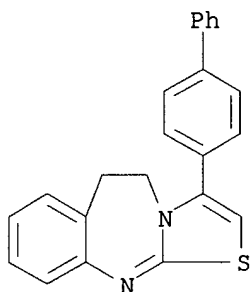
RN 318529-86-1 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-(2-furanyl)-5,6-dihydro- (9CI) (CA INDEX NAME)



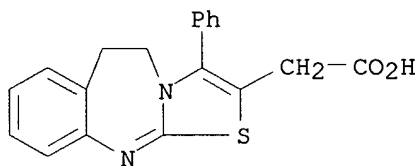
RN 318529-87-2 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-[1,1'-biphenyl]-4-yl-5,6-dihydro-,
monohydrochloride (9CI) (CA INDEX NAME)

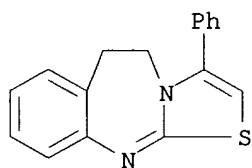


● HCl

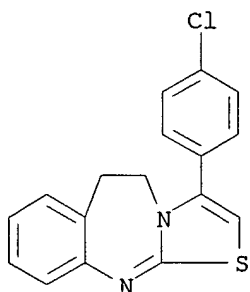
RN 318529-88-3 CAPLUS
 CN Thiazolo[2,3-b][1,3]benzodiazepine-2-acetic acid, 5,6-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



RN 318529-89-4 CAPLUS
 CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-phenyl- (9CI) (CA INDEX NAME)

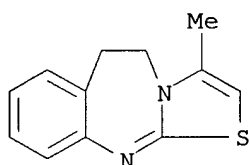


RN 318529-90-7 CAPLUS
 CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-(4-chlorophenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)



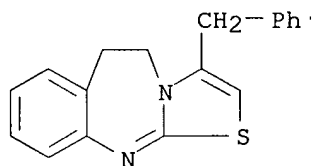
RN 318529-91-8 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-methyl- (9CI) (CA INDEX NAME)



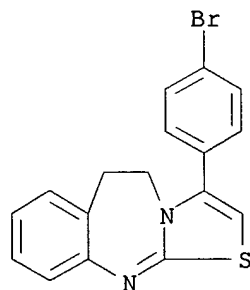
RN 318529-92-9 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 318529-93-0 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-(4-bromophenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)

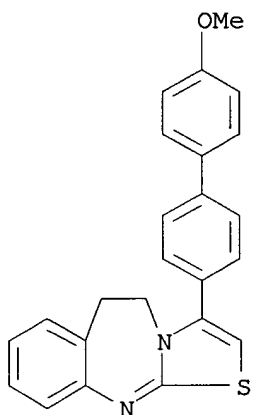


RN 318529-94-1 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(4'-methoxy[1,1'-

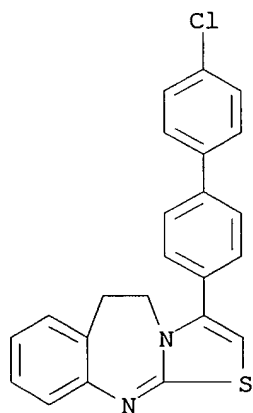
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biphenyl]-4-yl)- (9CI) (CA INDEX NAME)



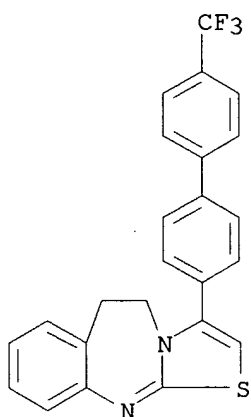
RN 318529-95-2 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-(4'-chloro[1,1'-biphenyl]-4-yl)-5,6-dihydro- (9CI) (CA INDEX NAME)



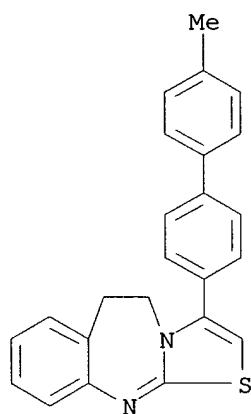
RN 318529-96-3 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-[4'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



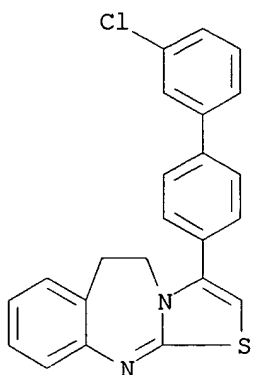
RN 318529-97-4 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(4'-methyl[1,1'-biphenyl]-4-yl)- (9CI) (CA INDEX NAME)



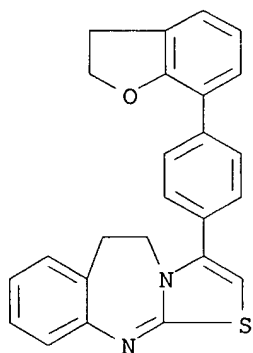
RN 318529-98-5 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-(3'-chloro[1,1'-biphenyl]-4-yl)-5,6-dihydro- (9CI) (CA INDEX NAME)



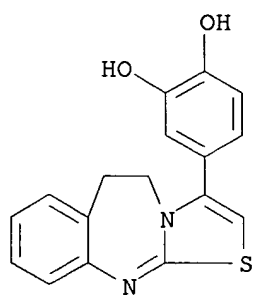
RN 318529-99-6 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-[4-(2,3-dihydro-7-benzofuranyl)phenyl]-5,6-dihydro- (9CI). (CA INDEX NAME)



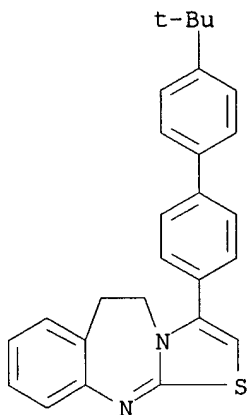
RN 318530-00-6 CAPLUS

CN 1,2-Benzenediol, 4-(5,6-dihydrothiazolo[2,3-b][1,3]benzodiazepin-3-yl)- (9CI) (CA INDEX NAME)

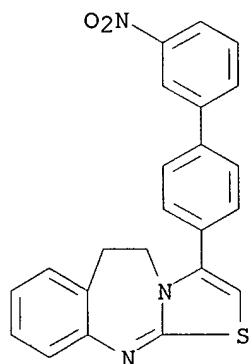


RN 318530-01-7 CAPLUS

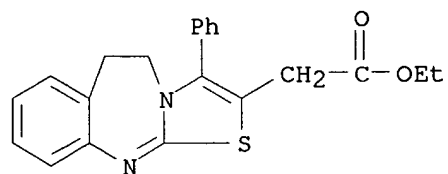
CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-[4'-(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl]-5,6-dihydro- (9CI) (CA INDEX NAME)



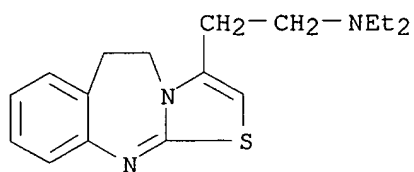
RN 318530-02-8 CAPLUS
 CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(3'-nitro[1,1'-biphenyl]-4-yl)- (9CI) (CA INDEX NAME)



RN 318530-03-9 CAPLUS
 CN Thiazolo[2,3-b][1,3]benzodiazepine-2-acetic acid, 5,6-dihydro-3-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

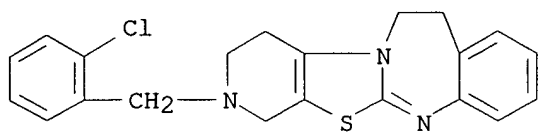


RN 318530-04-0 CAPLUS
 CN Thiazolo[2,3-b][1,3]benzodiazepine-3-ethanamine, N,N-diethyl-5,6-dihydro- (9CI) (CA INDEX NAME)



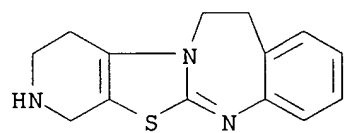
RN 318530-05-1 CAPLUS

CN Pyrido[4',3':4,5]thiazolo[2,3-b][1,3]benzodiazepine, 2-[(2-chlorophenyl)methyl]-1,2,3,4,6,7-hexahydro- (9CI) (CA INDEX NAME)



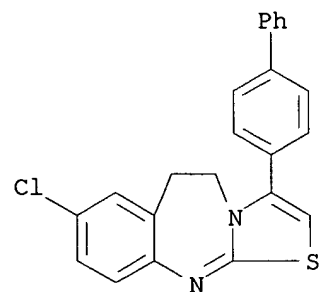
RN 318530-06-2 CAPLUS

CN Pyrido[4',3':4,5]thiazolo[2,3-b][1,3]benzodiazepine, 1,2,3,4,6,7-hexahydro- (9CI) (CA INDEX NAME)



RN 318530-07-3 CAPLUS

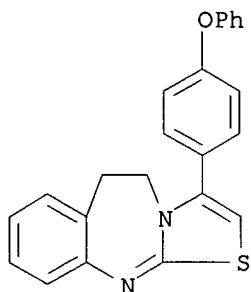
CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-[1,1'-biphenyl]-4-yl-8-chloro-5,6-dihydro- (9CI) (CA INDEX NAME)



RN 318530-08-4 CAPLUS

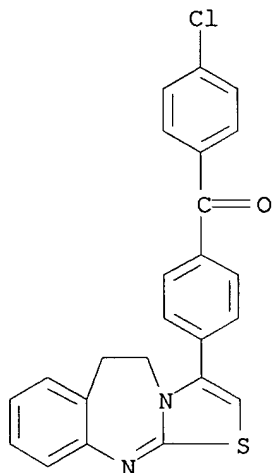
CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)

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RN 318530-09-5 CAPLUS

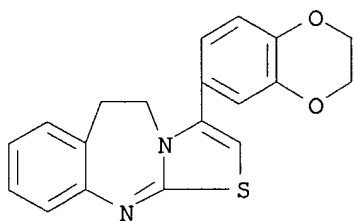
CN Methanone, (4-chlorophenyl) [4-(5,6-dihydrothiazolo[2,3-b][1,3]benzodiazepin-3-yl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

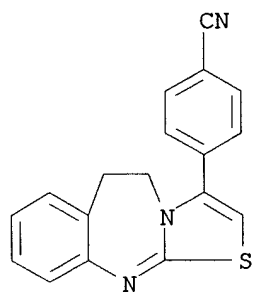
RN 318530-10-8 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-(2,3-dihydro-1,4-benzodioxin-6-yl)-5,6-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)



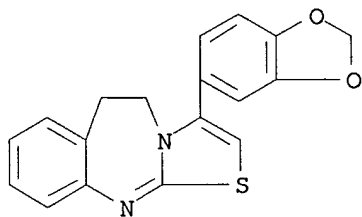
● HCl

RN 318530-11-9 CAPLUS
CN Benzonitrile, 4-(5,6-dihydrothiazolo[2,3-b][1,3]benzodiazepin-3-yl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

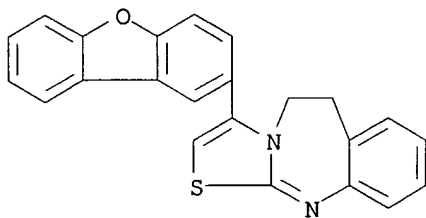
RN 318530-12-0 CAPLUS
CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-(1,3-benzodioxol-5-yl)-5,6-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

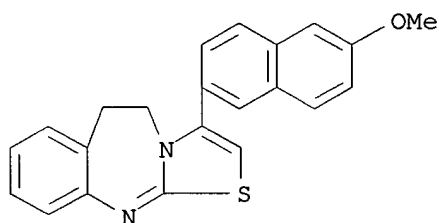
RN 318530-13-1 CAPLUS
CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-(2-dibenzofuranyl)-5,6-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

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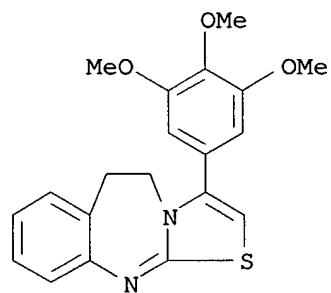
● HCl

RN 318530-14-2 CAPLUS
CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(6-methoxy-2-naphthalenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 318530-15-3 CAPLUS
CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(3,4,5-trimethoxyphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

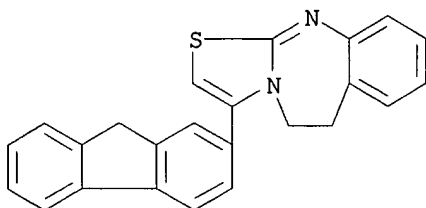


● HCl

RN 318530-16-4 CAPLUS
CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-(9H-fluoren-2-yl)-5,6-dihydro-,

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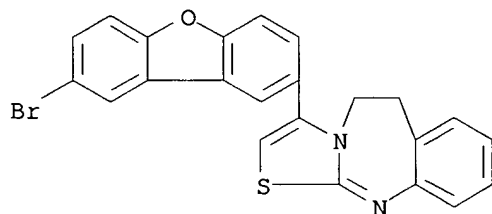
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 318530-17-5 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-(8-bromo-2-dibenzofuranyl)-5,6-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

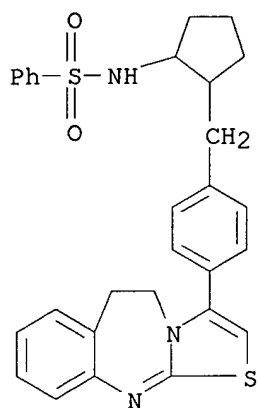


● HCl

RN 318530-18-6 CAPLUS

CN Benzenesulfonamide, N-[2-[[4-(5,6-dihydrothiazolo[2,3-b][1,3]benzodiazepin-3-yl)phenyl]methyl]cyclopentyl]-, monohydrochloride (9CI) (CA INDEX NAME)

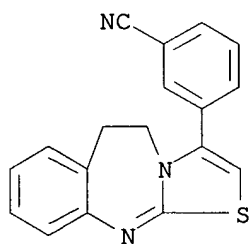
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● HCl

RN 318530-19-7 CAPLUS

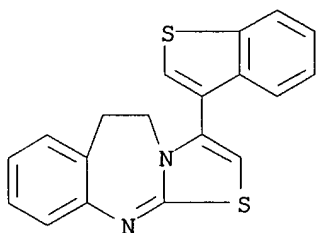
CN Benzonitrile, 3-(5,6-dihydrothiazolo[2,3-b][1,3]benzodiazepin-3-yl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 318530-20-0 CAPLUS

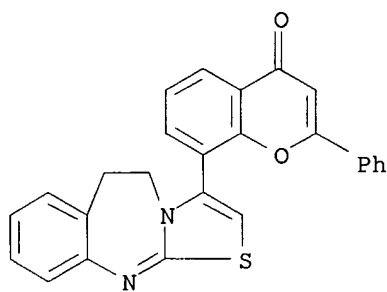
CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-benzo[b]thien-3-yl-5,6-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 318530-21-1 CAPLUS

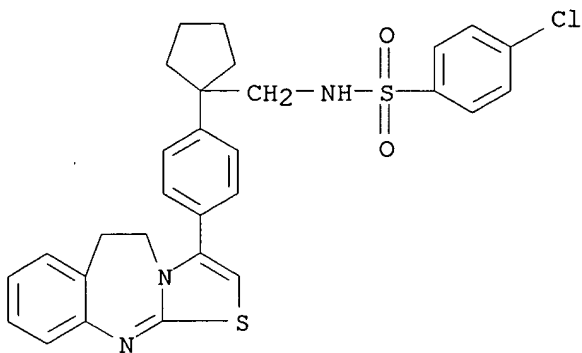
CN 4H-1-Benzopyran-4-one, 8-(5,6-dihydrothiazolo[2,3-b][1,3]benzodiazepin-3-yl)-2-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

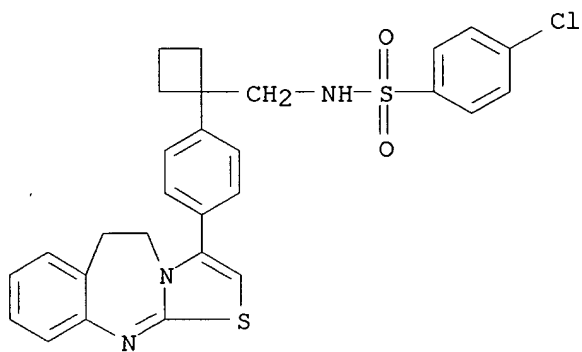
RN 318530-22-2 CAPLUS

CN Benzenesulfonamide, 4-chloro-N-[[1-[4-(5,6-dihydrothiazolo[2,3-b][1,3]benzodiazepin-3-yl)phenyl]cyclopentyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



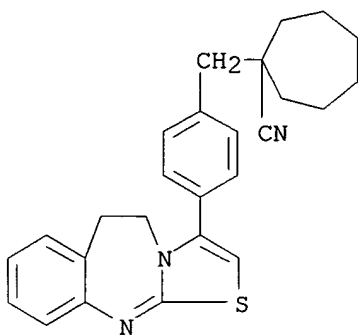
● HCl

RN 318530-23-3 CAPLUS
 CN Benzenesulfonamide, 4-chloro-N-[[1-[4-(5,6-dihydrothiazolo[2,3-b][1,3]benzodiazepin-3-yl)phenyl]cyclobutyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

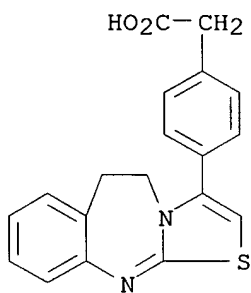
RN 318530-24-4 CAPLUS
 CN Cycloheptanecarbonitrile, 1-[[4-(5,6-dihydrothiazolo[2,3-b][1,3]benzodiazepin-3-yl)phenyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 318530-25-5 CAPLUS

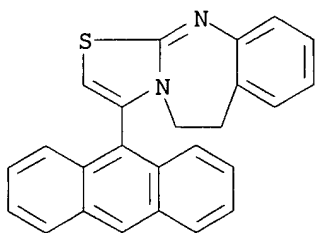
CN Benzeneacetic acid, 4-(5,6-dihydrothiazolo[2,3-b][1,3]benzodiazepin-3-yl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

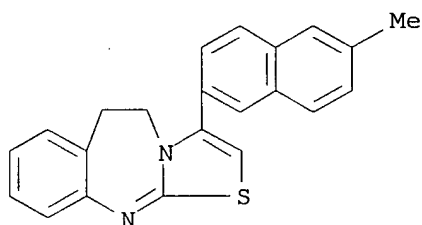
RN 318530-26-6 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-(9-anthracenyl)-5,6-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)



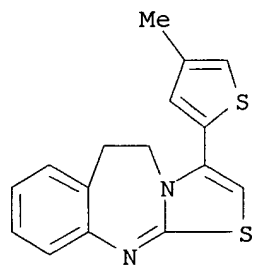
● HCl

RN 318530-27-7 CAPLUS
CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(6-methyl-2-naphthalenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

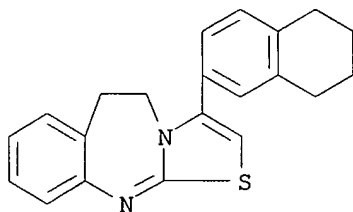
RN 318530-28-8 CAPLUS
CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(4-methyl-2-thienyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 318530-29-9 CAPLUS
CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(5,6,7,8-tetrahydro-2-naphthalenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

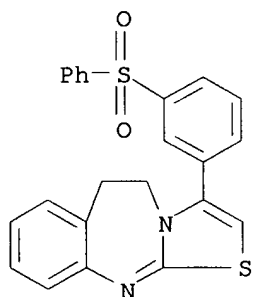
10/019,683



● HCl

RN 318530-30-2 CAPLUS

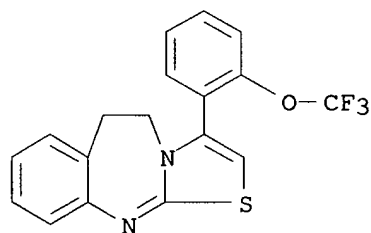
CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-[3-(phenylsulfonyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 318530-31-3 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-[2-(trifluoromethoxy)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

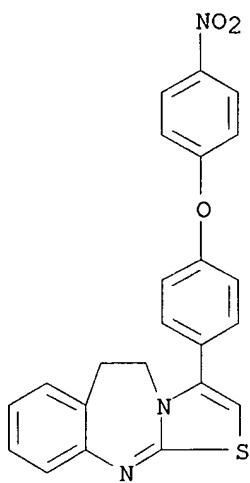


● HCl

RN 318530-32-4 CAPLUS

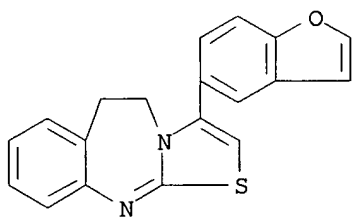
10/019,683

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-[4-(4-nitrophenoxy)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

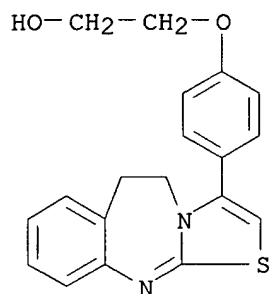
RN 318530-33-5 CAPLUS
CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-(5-benzofuranyl)-5,6-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 318530-34-6 CAPLUS
CN Ethanol, 2-[4-(5,6-dihydrothiazolo[2,3-b][1,3]benzodiazepin-3-yl)phenoxy]-, monohydrochloride (9CI) (CA INDEX NAME)

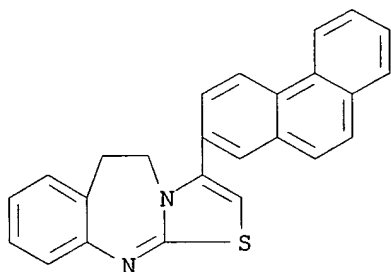
10/019,683



● HCl

RN 318530-35-7 CAPLUS

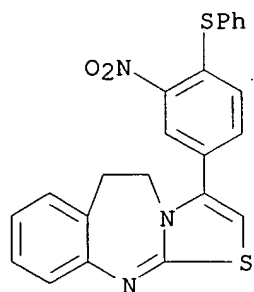
CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(2-phenanthrenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 318530-36-8 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-[3-nitro-4-(phenylthio)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

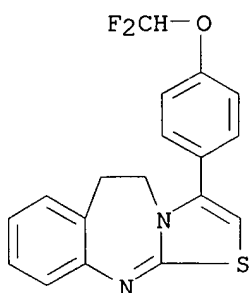
RN 318530-37-9 CAPLUS

CN 11H-Indeno[2',1':4,5]thiazolo[2,3-b][1,3]benzodiazepine, 13,14-dihydro-
(9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 318530-38-0 CAPLUS

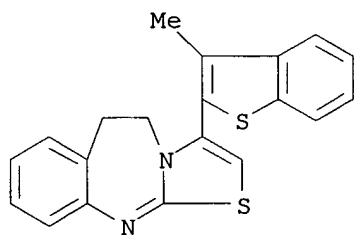
CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-[4-(difluoromethoxy)phenyl]-5,6-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 318530-39-1 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(3-methylbenzo[b]thien-2-yl)-, monohydrochloride (9CI) (CA INDEX NAME)

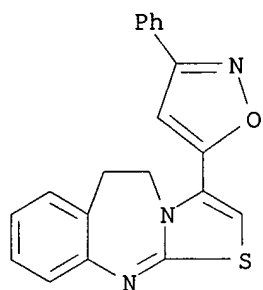


● HCl

RN 318530-40-4 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(3-phenyl-5-isoxazolyl)-, monohydrochloride (9CI) (CA INDEX NAME)

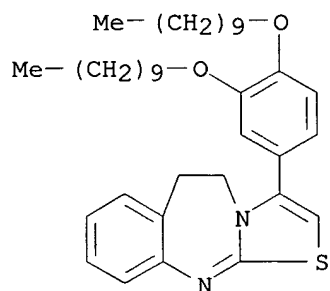
10/019,683



● HCl

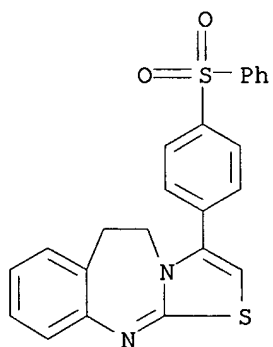
RN 318530-41-5 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-[3,4-bis(decyloxy)phenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)



RN 318530-42-6 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-[4-(phenylsulfonyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

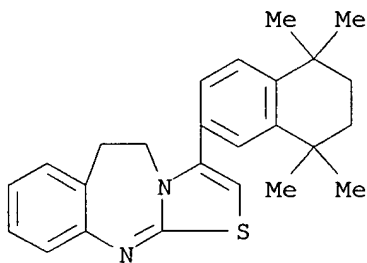


● HCl

RN 318530-43-7 CAPLUS

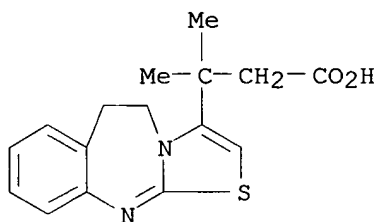
10/019,683

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)- (9CI) (CA INDEX NAME)



RN 318530-44-8 CAPLUS

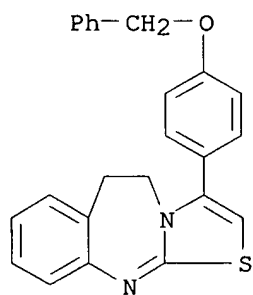
CN Thiazolo[2,3-b][1,3]benzodiazepine-3-propanoic acid, 5,6-dihydro- β,β -dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

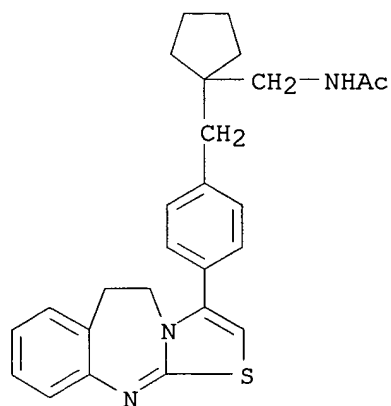
RN 318530-45-9 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-[4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)

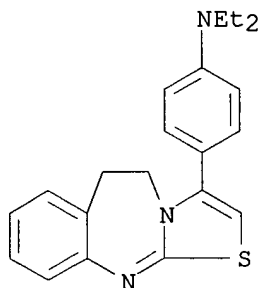


RN 318530-46-0 CAPLUS

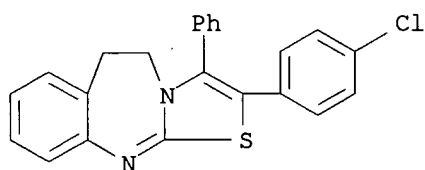
CN Acetamide, N-[[1-[[4-(5,6-dihydrothiazolo[2,3-b][1,3]benzodiazepin-3-yl)phenyl]methyl]cyclopentyl]methyl]- (9CI) (CA INDEX NAME)



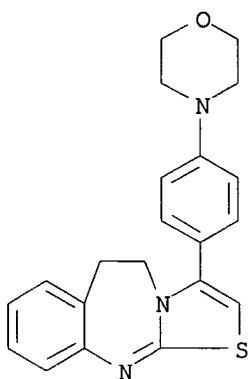
RN 318530-47-1 CAPLUS
 CN Benzenamine, 4-(5,6-dihydrothiazolo[2,3-b][1,3]benzodiazepin-3-yl)-N,N-diethyl- (9CI) (CA INDEX NAME)



RN 318530-48-2 CAPLUS
 CN Thiazolo[2,3-b][1,3]benzodiazepine, 2-(4-chlorophenyl)-5,6-dihydro-3-phenyl- (9CI) (CA INDEX NAME)

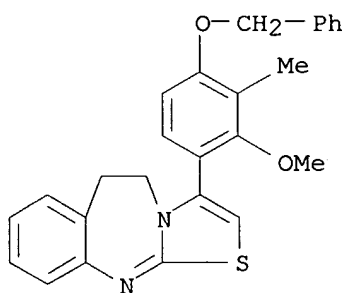


RN 318530-49-3 CAPLUS
 CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-[4-(4-morpholinyl)phenyl]- (9CI) (CA INDEX NAME)



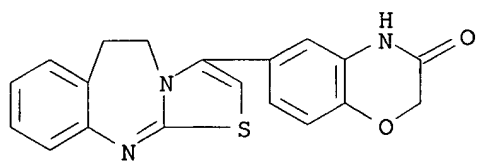
RN 318530-50-6 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-[2-methoxy-3-methyl-4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



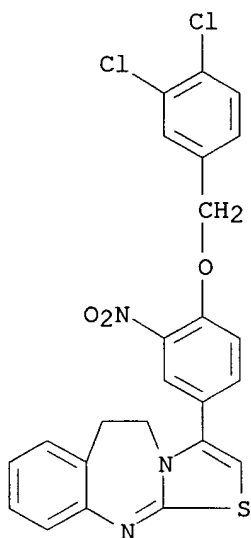
RN 318530-51-7 CAPLUS

CN 2H-1,4-Benzoxazin-3(4H)-one, 6-(5,6-dihydrothiazolo[2,3-b][1,3]benzodiazepin-3-yl)- (9CI) (CA INDEX NAME)



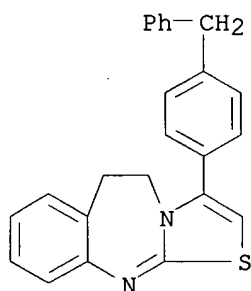
RN 318530-52-8 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-[4-[(3,4-dichlorophenyl)methoxy]-3-nitrophenyl]-5,6-dihydro- (9CI) (CA INDEX NAME)



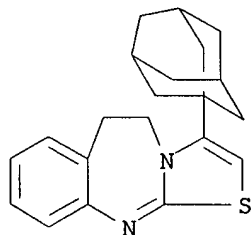
RN 318530-53-9 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-[4-(phenylmethyl)phenyl]-
(9CI) (CA INDEX NAME)



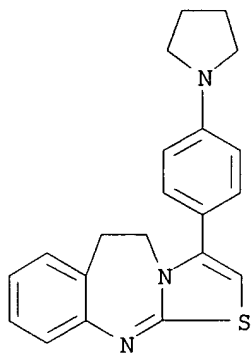
RN 318530-54-0 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-tricyclo[3.3.1.1^{3,7}]dec-
1-yl- (9CI) (CA INDEX NAME)



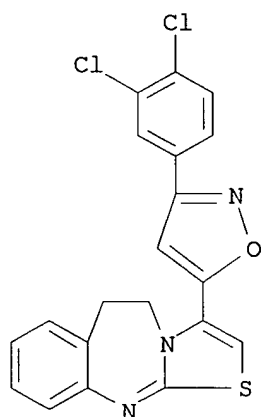
RN 318530-55-1 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-[4-(1-
pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



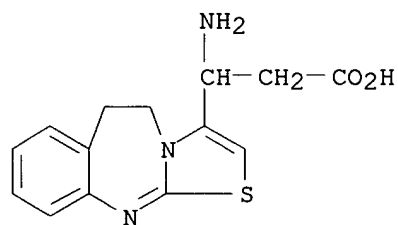
RN 318530-56-2 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-[3-(3,4-dichlorophenyl)-5-isoxazolyl]-5,6-dihydro- (9CI) (CA INDEX NAME)



RN 318530-57-3 CAPLUS

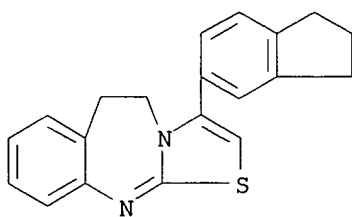
CN Thiazolo[2,3-b][1,3]benzodiazepine-3-propanoic acid, β -amino-5,6-dihydro- (9CI) (CA INDEX NAME)



RN 318530-58-4 CAPLUS

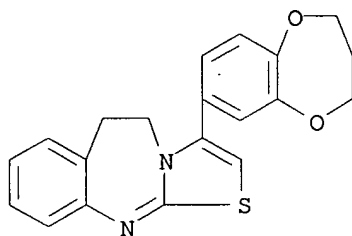
CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-(2,3-dihydro-1H-inden-5-yl)-5,6-dihydro- (9CI) (CA INDEX NAME)

10/019,683



RN 318530-59-5 CAPLUS

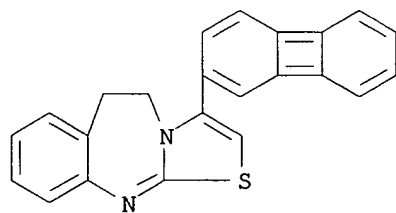
CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-(3,4-dihydro-2H-1,5-benzodioxepin-7-yl)-5,6-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

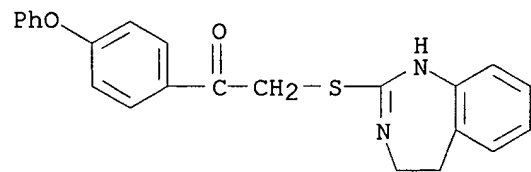
RN 318530-60-8 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 3-(2-biphenylenyl)-5,6-dihydro- (9CI) (CA INDEX NAME)



RN 318530-61-9 CAPLUS

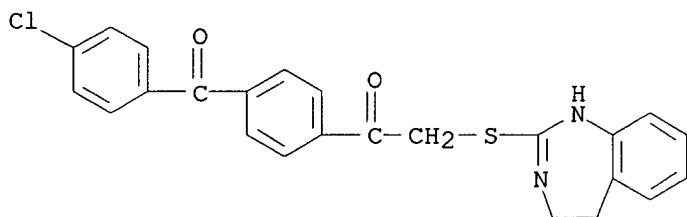
CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)



10/019,683

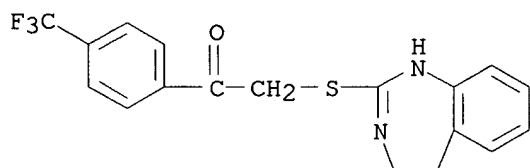
RN 318530-62-0 CAPLUS

CN Ethanone, 1-[4-(4-chlorobenzoyl)phenyl]-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



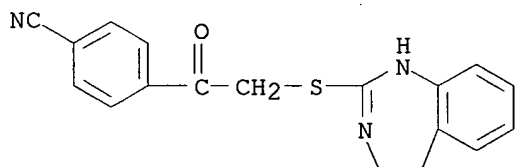
RN 318530-63-1 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



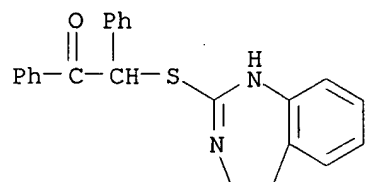
RN 318530-64-2 CAPLUS

CN Benzonitrile, 4-[[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]acetyl]- (9CI) (CA INDEX NAME)



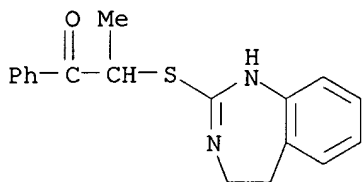
RN 318530-65-3 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1,2-diphenyl- (9CI) (CA INDEX NAME)



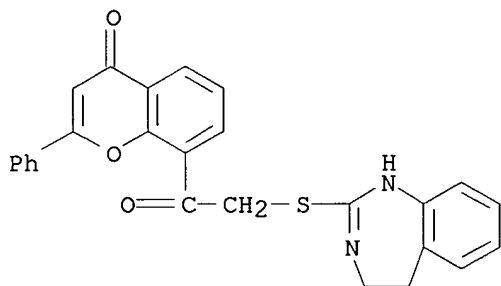
RN 318530-66-4 CAPLUS

CN 1-Propanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-phenyl- (9CI) (CA INDEX NAME)



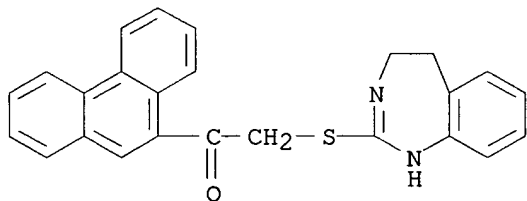
RN 318530-67-5 CAPLUS

CN 4H-1-Benzopyran-4-one, 8-[[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]acetyl]-2-phenyl- (9CI) (CA INDEX NAME)



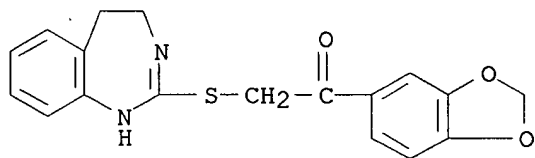
RN 318530-68-6 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(9-phenanthrenyl)- (9CI) (CA INDEX NAME)



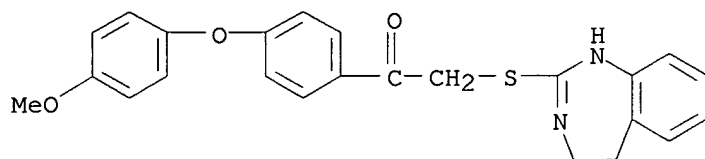
RN 318530-69-7 CAPLUS

CN Ethanone, 1-(1,3-benzodioxol-5-yl)-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



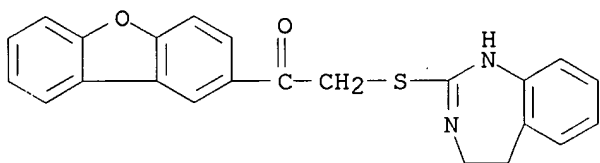
RN 318530-70-0 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-[4-(4-methoxyphenoxy)phenyl]- (9CI) (CA INDEX NAME)



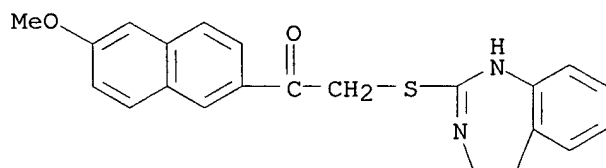
RN 318530-71-1 CAPLUS

CN Ethanone, 1-(2-dibenzofuranyl)-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



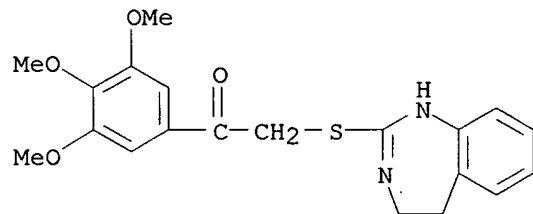
RN 318530-72-2 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(6-methoxy-2-naphthalenyl)- (9CI) (CA INDEX NAME)



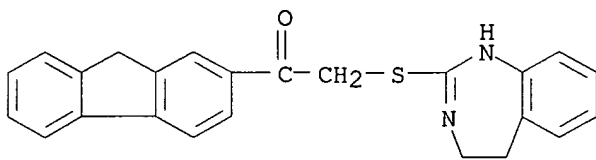
RN 318530-73-3 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)



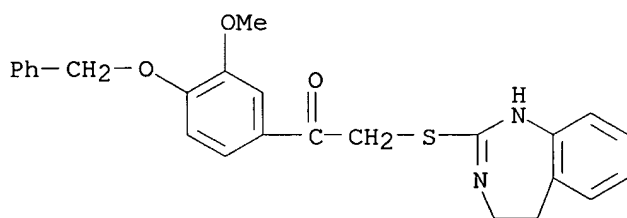
RN 318530-74-4 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(9H-fluoren-2-yl)- (9CI) (CA INDEX NAME)



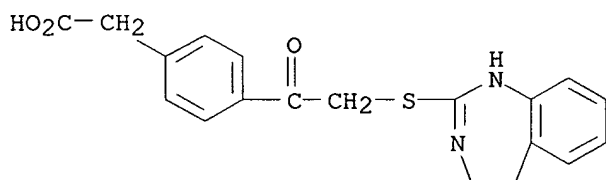
RN 318530-75-5 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-[3-methoxy-4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



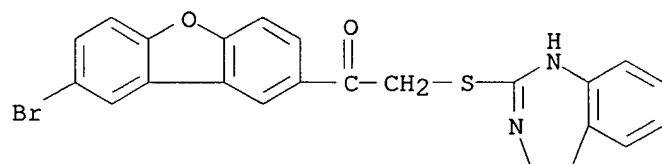
RN 318530-76-6 CAPLUS

CN Benzeneacetic acid, 4-[[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]acetyl]- (9CI) (CA INDEX NAME)



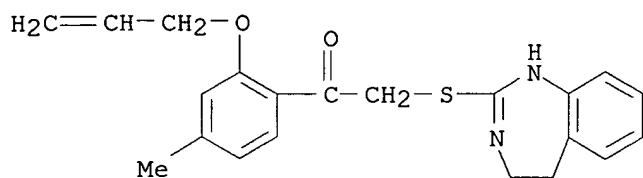
RN 318530-77-7 CAPLUS

CN Ethanone, 1-(8-bromo-2-dibenzofuranyl)-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



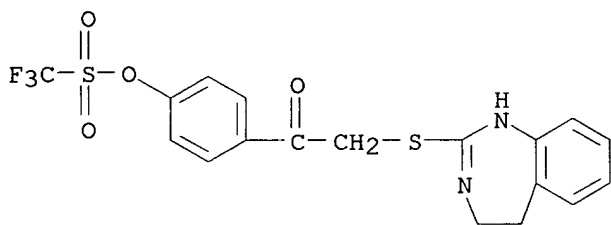
RN 318530-78-8 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-[4-methyl-2-(2-propenyloxy)phenyl]- (9CI) (CA INDEX NAME)



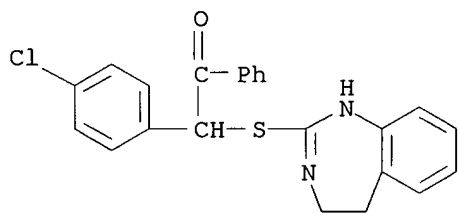
RN 318530-79-9 CAPLUS

CN Methanesulfonic acid, trifluoro-, 4-[[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]acetyl]phenyl ester (9CI) (CA INDEX NAME)



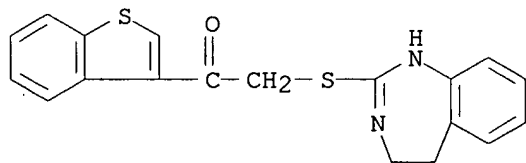
RN 318530-80-2 CAPLUS

CN Ethanone, 2-(4-chlorophenyl)-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-phenyl- (9CI) (CA INDEX NAME)



RN 318530-81-3 CAPLUS

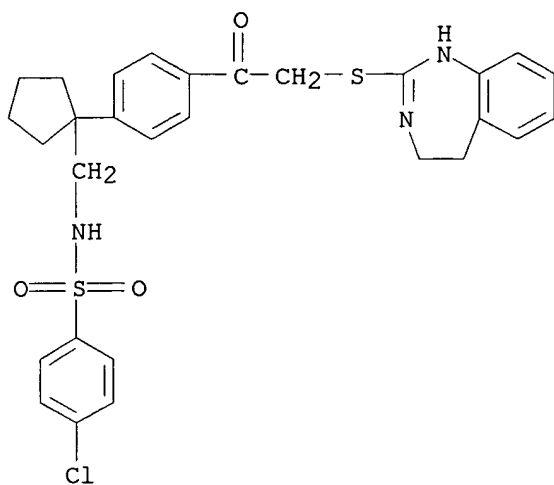
CN Ethanone, 1-benzo[b]thien-3-yl-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



RN 318530-82-4 CAPLUS

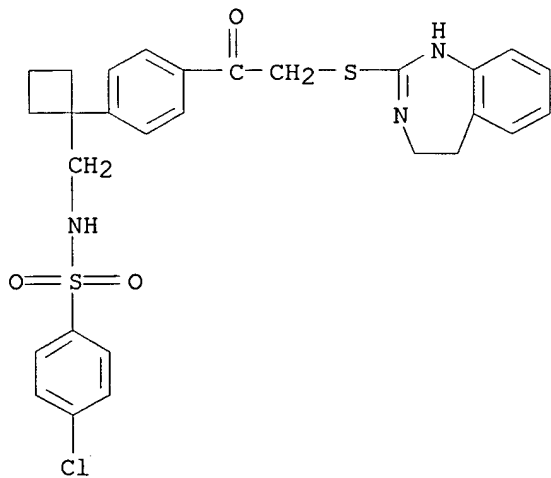
CN Benzenesulfonamide, 4-chloro-N-[[1-[4-[[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]acetyl]phenyl]cyclopentyl]methyl]- (9CI) (CA INDEX NAME)

1998, 1999, 2000, 2001, 2002, 2003, 2004, 2005, 2006, 2007, 2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015, 2016, 2017, 2018, 2019, 2020, 2021, 2022, 2023, 2024, 2025, 2026, 2027, 2028, 2029, 2030, 2031, 2032, 2033, 2034, 2035, 2036, 2037, 2038, 2039, 2040, 2041, 2042, 2043, 2044, 2045, 2046, 2047, 2048, 2049, 2050, 2051, 2052, 2053, 2054, 2055, 2056, 2057, 2058, 2059, 2060, 2061, 2062, 2063, 2064, 2065, 2066, 2067, 2068, 2069, 2070, 2071, 2072, 2073, 2074, 2075, 2076, 2077, 2078, 2079, 2080, 2081, 2082, 2083, 2084, 2085, 2086, 2087, 2088, 2089, 2090, 2091, 2092, 2093, 2094, 2095, 2096, 2097, 2098, 2099, 2100, 2101, 2102, 2103, 2104, 2105, 2106, 2107, 2108, 2109, 2110, 2111, 2112, 2113, 2114, 2115, 2116, 2117, 2118, 2119, 2120, 2121, 2122, 2123, 2124, 2125, 2126, 2127, 2128, 2129, 2130, 2131, 2132, 2133, 2134, 2135, 2136, 2137, 2138, 2139, 2140, 2141, 2142, 2143, 2144, 2145, 2146, 2147, 2148, 2149, 2150, 2151, 2152, 2153, 2154, 2155, 2156, 2157, 2158, 2159, 2160, 2161, 2162, 2163, 2164, 2165, 2166, 2167, 2168, 2169, 2170, 2171, 2172, 2173, 2174, 2175, 2176, 2177, 2178, 2179, 2180, 2181, 2182, 2183, 2184, 2185, 2186, 2187, 2188, 2189, 2190, 2191, 2192, 2193, 2194, 2195, 2196, 2197, 2198, 2199, 2200, 2201, 2202, 2203, 2204, 2205, 2206, 2207, 2208, 2209, 2210, 2211, 2212, 2213, 2214, 2215, 2216, 2217, 2218, 2219, 2220, 2221, 2222, 2223, 2224, 2225, 2226, 2227, 2228, 2229, 2230, 2231, 2232, 2233, 2234, 2235, 2236, 2237, 2238, 2239, 2240, 2241, 2242, 2243, 2244, 2245, 2246, 2247, 2248, 2249, 2250, 2251, 2252, 2253, 2254, 2255, 2256, 2257, 2258, 2259, 2260, 2261, 2262, 2263, 2264, 2265, 2266, 2267, 2268, 2269, 2270, 2271, 2272, 2273, 2274, 2275, 2276, 2277, 2278, 2279, 2280, 2281, 2282, 2283, 2284, 2285, 2286, 2287, 2288, 2289, 2290, 2291, 2292, 2293, 2294, 2295, 2296, 2297, 2298, 2299, 2300, 2301, 2302, 2303, 2304, 2305, 2306, 2307, 2308, 2309, 2310, 2311, 2312, 2313, 2314, 2315, 2316, 2317, 2318, 2319, 2320, 2321, 2322, 2323, 2324, 2325, 2326, 2327, 2328, 2329, 2330, 2331, 2332, 2333, 2334, 2335, 2336, 2337, 2338, 2339, 2340, 2341, 2342, 2343, 2344, 2345, 2346, 2347, 2348, 2349, 2350, 2351, 2352, 2353, 2354, 2355, 2356, 2357, 2358, 2359, 2360, 2361, 2362, 2363, 2364, 2365, 2366, 2367, 2368, 2369, 2370, 2371, 2372, 2373, 2374, 2375, 2376, 2377, 2378, 2379, 2380, 2381, 2382, 2383, 2384, 2385, 2386, 2387, 2388, 2389, 2390, 2391, 2392, 2393, 2394, 2395, 2396, 2397, 2398, 2399, 2400, 2401, 2402, 2403, 2404, 2405, 2406, 2407, 2408, 2409, 2410, 2411, 2412, 2413, 2414, 2415, 2416, 2417, 2418, 2419, 2420, 2421, 2422, 2423, 2424, 2425, 2426, 2427, 2428, 2429, 2430, 2431, 2432, 2433, 2434, 2435, 2436, 2437, 2438, 2439, 2440, 2441, 2442, 2443, 2444, 2445, 2446, 2447, 2448, 2449, 2450, 2451, 2452, 2453, 2454, 2455, 2456, 2457, 2458, 2459, 2460, 2461, 2462, 2463, 2464, 2465, 2466, 2467, 2468, 2469, 2470, 2471, 2472, 2473, 2474, 2475, 2476, 2477, 2478, 2479, 2480, 2481, 2482, 2483, 2484, 2485, 2486, 2487, 2488, 2489, 2490, 2491, 2492, 2493, 2494, 2495, 2496, 2497, 2498, 2499, 2500, 2501, 2502, 2503, 2504, 2505, 2506, 2507, 2508, 2509, 2510, 2511, 2512, 2513, 2514, 2515, 2516, 2517, 2518, 2519, 2520, 2521, 2522, 2523, 2524, 2525, 2526, 2527, 2528, 2529, 2530, 2531, 2532, 2533, 2534, 2535, 2536, 2537, 2538, 2539, 2540, 2541, 2542, 2543, 2544, 2545, 2546, 2547, 2548, 2549, 2550, 2551, 2552, 2553, 2554, 2555, 2556, 2557, 2558, 2559, 2560, 2561, 2562, 2563, 2564, 2565, 2566, 2567, 2568, 2569, 2570, 2571, 2572, 2573, 2574, 2575, 2576, 2577, 2578, 2579, 2580, 2581, 2582, 2583, 2584, 2585, 2586, 2587, 2588, 2589, 2590, 2591, 2592, 2593, 2594, 2595, 2596, 2597, 2598, 2599, 2600, 2601, 2602, 2603, 2604, 2605, 2606, 2607, 2608, 2609, 2610, 2611, 2612, 2613, 2614, 2615, 2616, 2617, 2618, 2619, 2620, 2621, 2622, 2623, 2624, 2625, 2626, 2627, 2628, 2629, 2630, 2631, 2632, 2633, 2634, 2635, 2636, 2637, 2638, 2639, 2640, 2641, 2642, 2643, 2644, 2645, 2646, 2647, 2648, 2649, 2650, 2651, 2652, 2653, 2654, 2655, 2656, 2657, 2658, 2659, 2660, 2661, 2662, 2663, 2664, 2665, 2666, 2667, 2668, 2669, 2670, 2671, 2672, 2673, 2674, 2675, 2676, 2677, 2678, 2679, 26



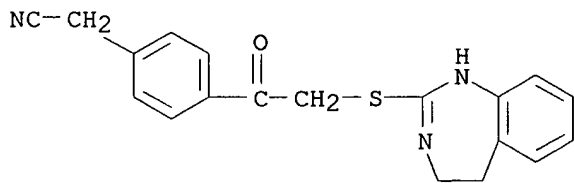
RN 318530-83-5 CAPLUS

Benzenesulfonamide, 4-chloro-N-[[[1-[4-[[[4,5-dihydro-1H-1,3-benzodiazepin-2-yl]thio]acetyl]phenyl]cyclobutyl]methyl]- (9CI) (CA INDEX NAME)



RN 318530-84-6 CAPLUS

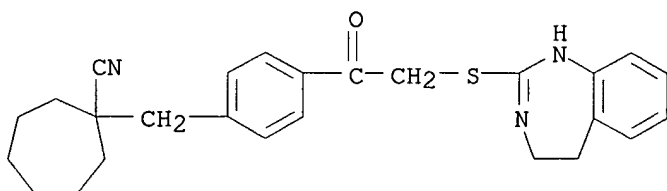
CN Benzeneacetonitrile, 4-[[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]acetyl]- (9CI) (CA INDEX NAME)



RN 318530-85-7 CAPLUS

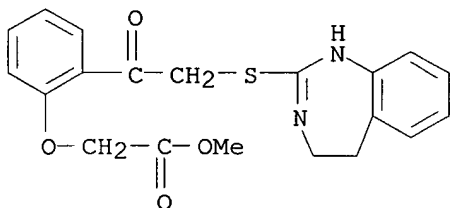
10/019,683

CN Cycloheptanecarbonitrile, 1-[[4-[[[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]acetyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



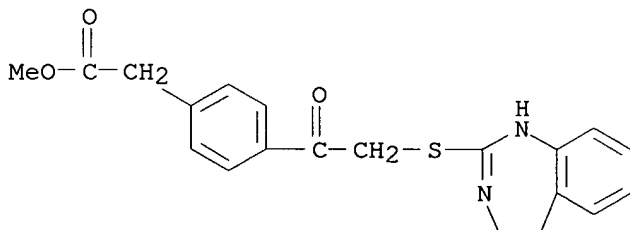
RN 318530-86-8 CAPLUS

CN Acetic acid, [2-[[[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]acetyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)



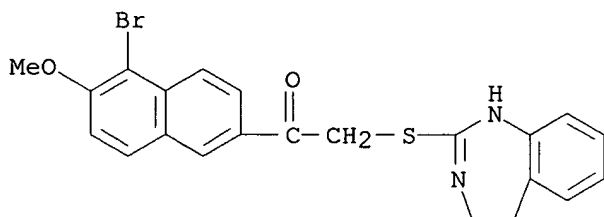
RN 318530-87-9 CAPLUS

CN Benzeneacetic acid, 4-[[[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]acetyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 318530-88-0 CAPLUS

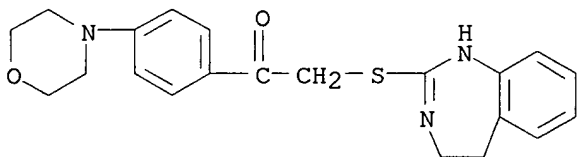
CN Ethanone, 1-(5-bromo-6-methoxy-2-naphthalenyl)-2-[[[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



10/019,683

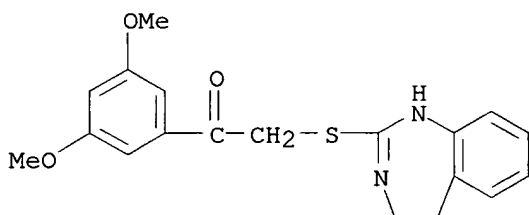
RN 318530-89-1 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-[4-(4-morpholinyl)phenyl]- (9CI) (CA INDEX NAME)



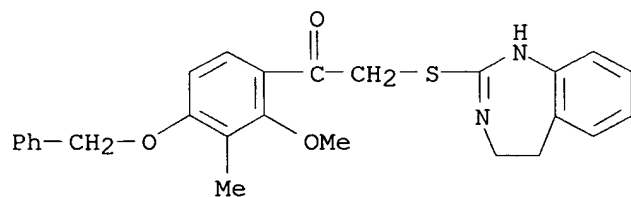
RN 318530-90-4 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(3,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



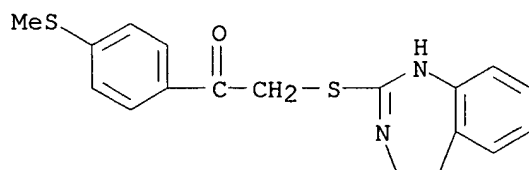
RN 318530-91-5 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-[2-methoxy-3-methyl-4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



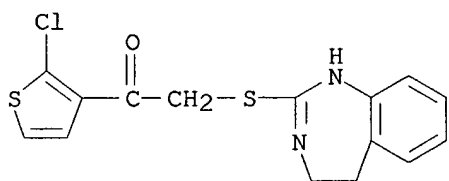
RN 318530-92-6 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-[4-(methylthio)phenyl]- (9CI) (CA INDEX NAME)



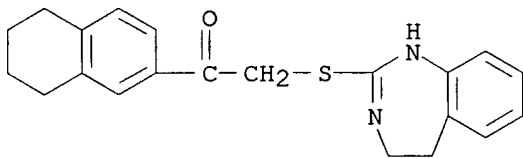
RN 318530-93-7 CAPLUS

CN Ethanone, 1-(2-chloro-3-thienyl)-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



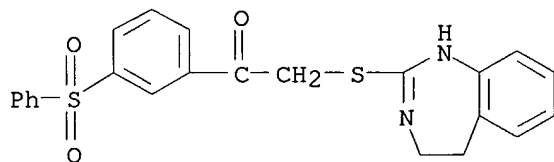
RN 318530-94-8 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(5,6,7,8-tetrahydro-2-naphthalenyl)- (9CI) (CA INDEX NAME)



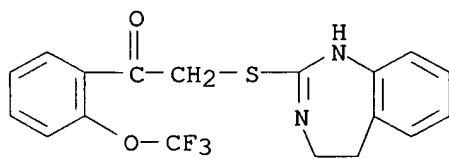
RN 318530-95-9 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-[3-(phenylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



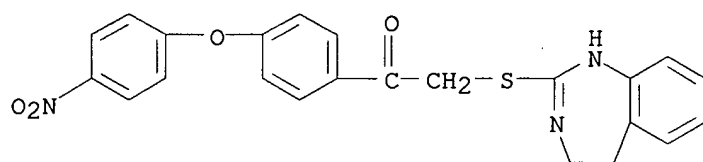
RN 318530-96-0 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-[2-(trifluoromethoxy)phenyl]- (9CI) (CA INDEX NAME)



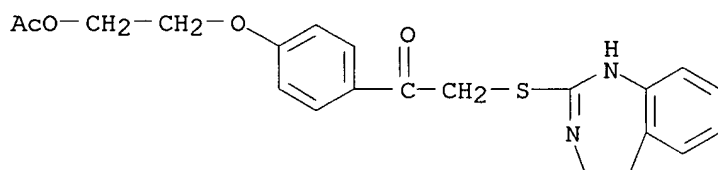
RN 318530-97-1 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-[4-(4-nitrophenoxy)phenyl]- (9CI) (CA INDEX NAME)



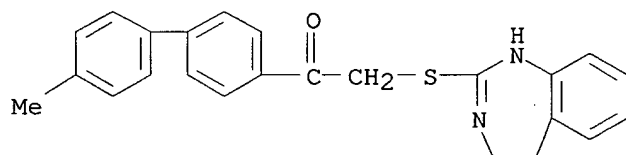
RN 318530-98-2 CAPLUS

CN Ethanone, 1-[4-[2-(acetyloxy)ethoxy]phenyl]-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



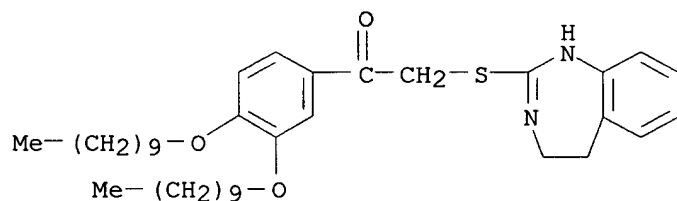
RN 318530-99-3 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(4'-methyl[1,1'-biphenyl]-4-yl)- (9CI) (CA INDEX NAME)



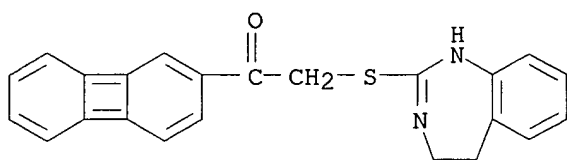
RN 318531-00-9 CAPLUS

CN Ethanone, 1-[3,4-bis(decyloxy)phenyl]-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



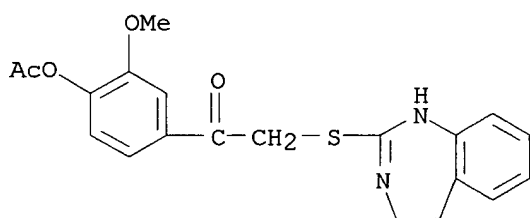
RN 318531-01-0 CAPLUS

CN Ethanone, 1-(2-biphenylenyl)-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



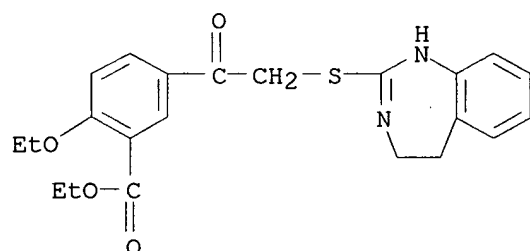
RN 318531-02-1 CAPLUS

CN Ethanone, 1-[4-(acetyloxy)-3-methoxyphenyl]-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



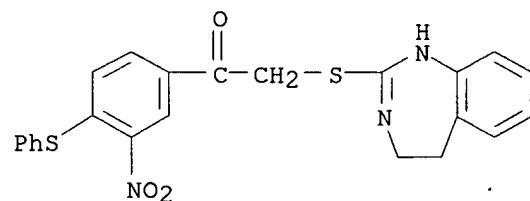
RN 318531-03-2 CAPLUS

CN Benzoic acid, 5-[[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]acetyl]-2-ethoxy-, ethyl ester (9CI) (CA INDEX NAME)



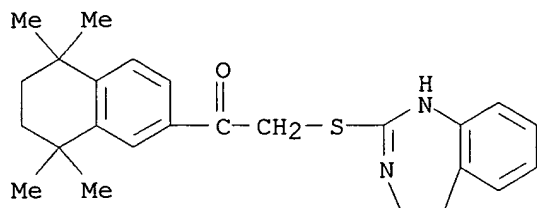
RN 318531-04-3 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-[3-nitro-4-(phenylthio)phenyl]- (9CI) (CA INDEX NAME)



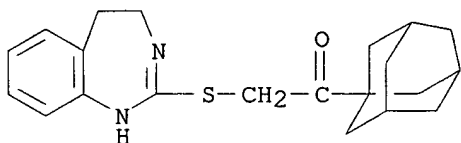
RN 318531-05-4 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)- (9CI) (CA INDEX NAME)



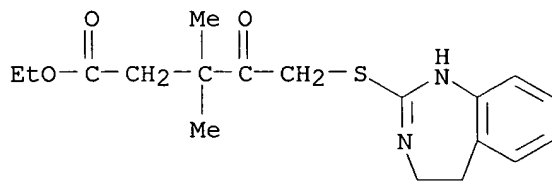
RN 318531-06-5 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-tricyclo[3.3.1.1.3,7]dec-1-yl- (9CI) (CA INDEX NAME)



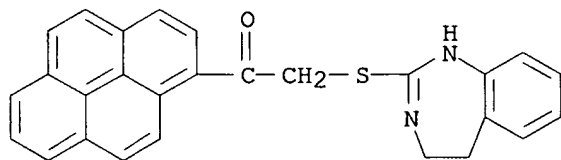
RN 318531-07-6 CAPLUS

CN Pentanoic acid, 5-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-3,3-dimethyl-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



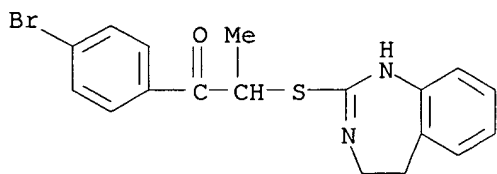
RN 318531-08-7 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(1-pyrenyl)- (9CI) (CA INDEX NAME)

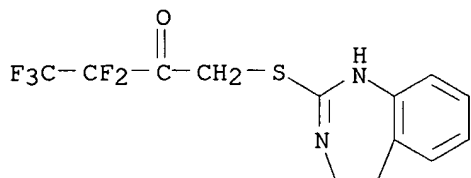


RN 318531-09-8 CAPLUS

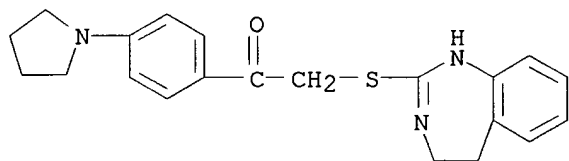
CN 1-Propanone, 1-(4-bromophenyl)-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



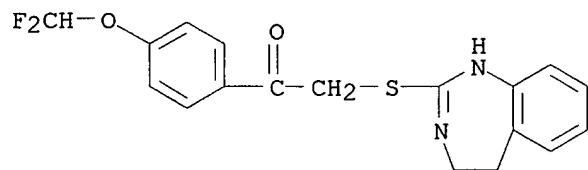
RN 318531-10-1 CAPLUS
 CN 2-Butanone, 1-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-3,3,4,4,4-pentafluoro- (9CI) (CA INDEX NAME)



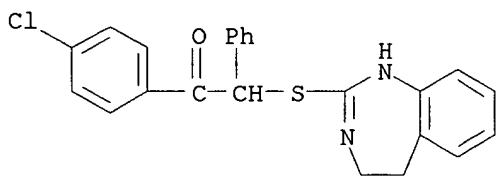
RN 318531-11-2 CAPLUS
 CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-[4-(1-pyrrolidinyl)phenyl]- (9CI) (CA INDEX NAME)



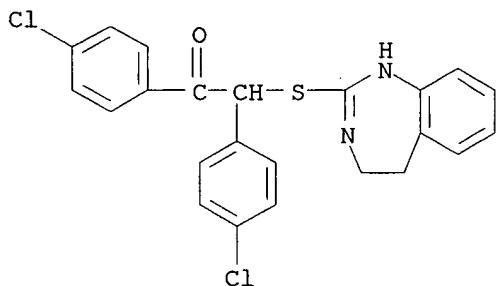
RN 318531-12-3 CAPLUS
 CN Ethanone, 1-[4-(difluoromethoxy)phenyl]-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



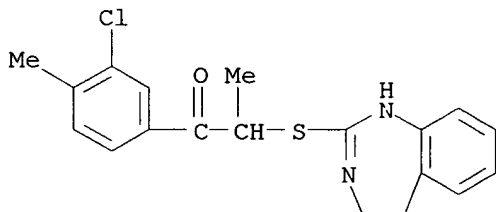
RN 318531-13-4 CAPLUS
 CN Ethanone, 1-(4-chlorophenyl)-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-2-phenyl- (9CI) (CA INDEX NAME)



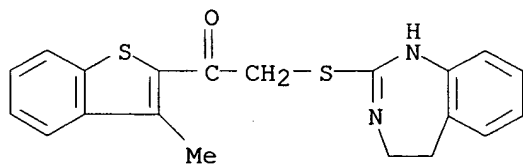
RN 318531-14-5 CAPLUS
 CN Ethanone, 1,2-bis(4-chlorophenyl)-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



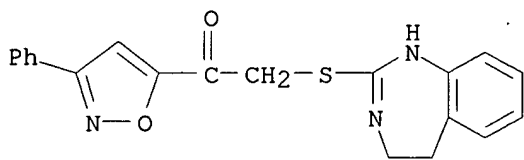
RN 318531-15-6 CAPLUS
 CN 1-Propanone, 1-(3-chloro-4-methylphenyl)-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



RN 318531-16-7 CAPLUS
 CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(3-methylbenzo[b]thien-2-yl)- (9CI) (CA INDEX NAME)

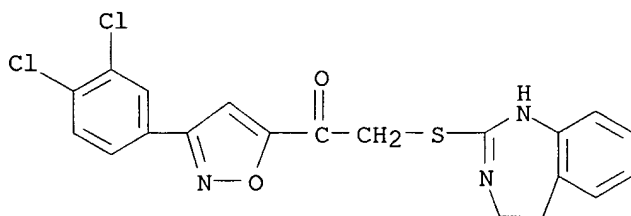


RN 318531-17-8 CAPLUS
 CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(3-phenyl-5-isoxazolyl)- (9CI) (CA INDEX NAME)



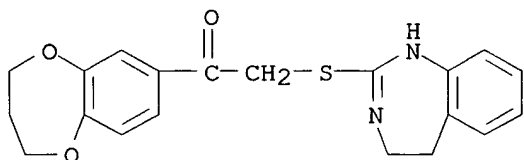
RN 318531-18-9 CAPLUS

CN Ethanone, 1-[3-(3,4-dichlorophenyl)-5-isoxazolyl]-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



RN 318531-19-0 CAPLUS

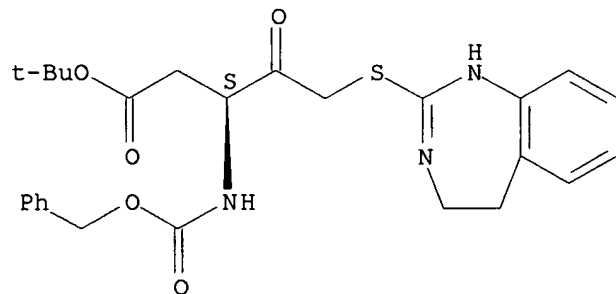
CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(3,4-dihydro-2H-1,5-benzodioxepin-7-yl)- (9CI) (CA INDEX NAME)



RN 318531-20-3 CAPLUS

CN Pentanoic acid, 5-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-4-oxo-3-[[(phenylmethoxy) carbonyl] amino]-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

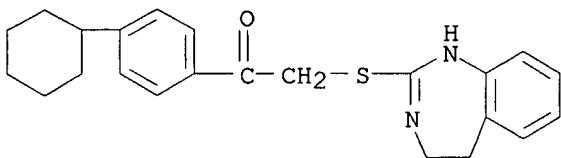
Absolute stereochemistry.



RN 318531-21-4 CAPLUS

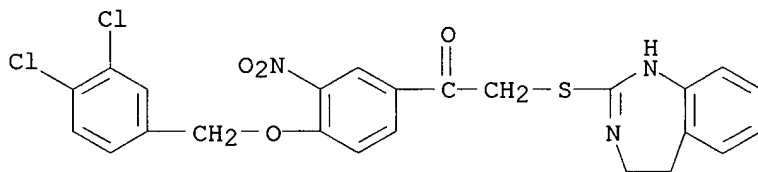
CN Ethanone, 1-(4-cyclohexylphenyl)-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-

yl)thio]- (9CI) (CA INDEX NAME)



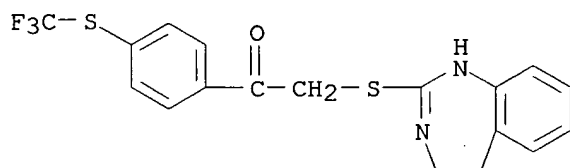
RN 318531-22-5 CAPLUS

CN Ethanone, 1-[4-[(3,4-dichlorophenyl)methoxy]-3-nitrophenyl]-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



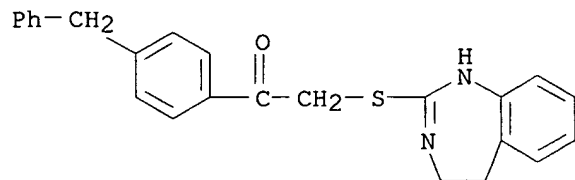
RN 318531-23-6 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-[4-[(trifluoromethyl)thio]phenyl]- (9CI) (CA INDEX NAME)



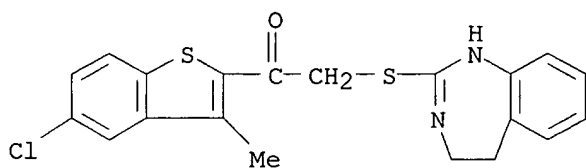
RN 318531-24-7 CAPLUS

CN Ethanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-[4-(phenylmethyl)phenyl]- (9CI) (CA INDEX NAME)



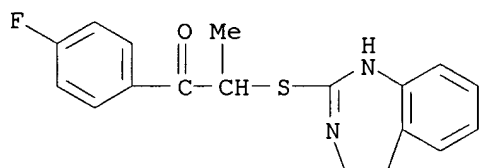
RN 318531-25-8 CAPLUS

CN Ethanone, 1-(5-chloro-3-methylbenzo[b]thien-2-yl)-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



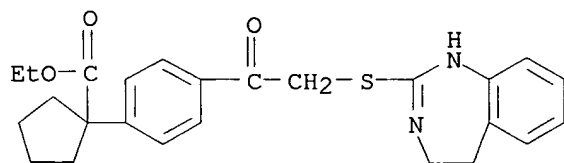
RN 318531-26-9 CAPLUS

CN 1-Propanone, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-1-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



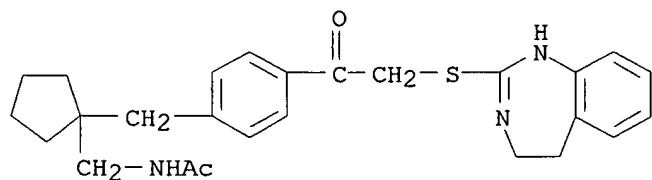
RN 318531-27-0 CAPLUS

CN Cyclopentanecarboxylic acid, 1-[4-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]acetyl]phenyl]-, ethyl ester (9CI) (CA INDEX NAME)



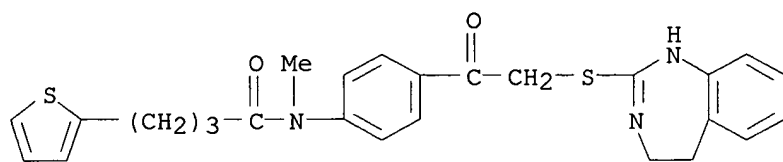
RN 318531-28-1 CAPLUS

CN Acetamide, N-[1-[4-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]acetyl]phenyl]methyl]cyclopentyl]methyl]- (9CI) (CA INDEX NAME)



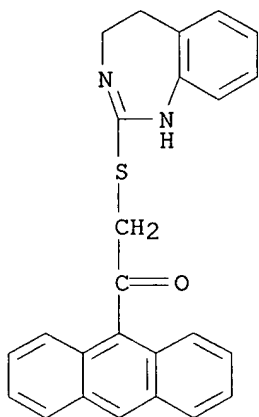
RN 318531-29-2 CAPLUS

CN 2-Thiophenebutanamide, N-[4-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]acetyl]phenyl]-N-methyl- (9CI) (CA INDEX NAME)



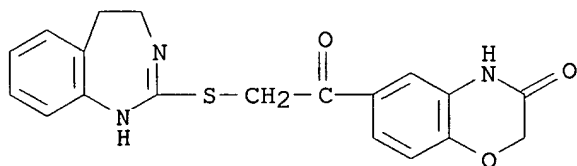
RN 318531-30-5 CAPLUS

CN Ethanone, 1-(9-anthracenyl)-2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]- (9CI) (CA INDEX NAME)



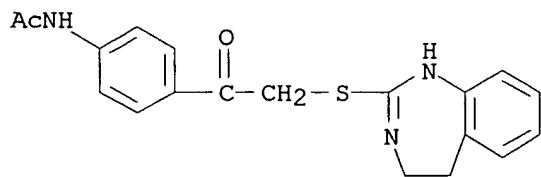
RN 318531-31-6 CAPLUS

CN 2H-1,4-Benzoxazin-3(4H)-one, 6-[[[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]acetyl]- (9CI) (CA INDEX NAME)



RN 318531-32-7 CAPLUS

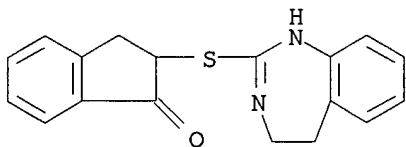
CN Acetamide, N-[4-[[[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]acetyl]phenyl]- (9CI) (CA INDEX NAME)



RN 318531-33-8 CAPLUS

10/019,683

CN 1H-Inden-1-one, 2-[(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)thio]-2,3-dihydro- (9CI) (CA INDEX NAME)

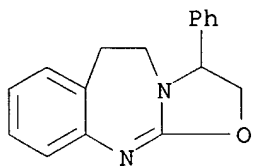


IT 88519-33-9P 318531-39-4P 318531-40-7P
318531-41-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dihydrobenzodiazepines and their use for treating dyslipidemia)

RN 88519-33-9 CAPLUS

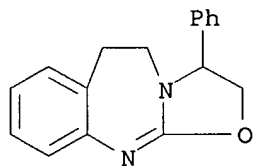
CN Oxazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-3-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

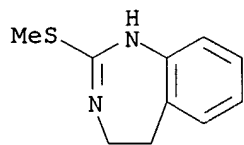
RN 318531-39-4 CAPLUS

CN Oxazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-3-phenyl- (9CI) (CA INDEX NAME)



RN 318531-40-7 CAPLUS

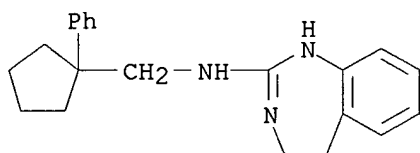
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(methylthio)- (9CI) (CA INDEX NAME)



10/019,683

RN 318531-41-8 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-[(1-phenylcyclopentyl)methyl]-
(9CI) (CA INDEX NAME)



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/019,683

~~LHA~~ ANSWER 6 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:355752 CAPLUS

DOCUMENT NUMBER: 131:719

TITLE: A covalent conjugate of clozapine with a fatty acid and its use for treating schizophrenia

INVENTOR(S): Bradley, Matthews O.; Shashoua, Victor E.; Swindell, Charles S.; Webb, Nigel L.

PATENT ASSIGNEE(S): Neuromedica, Inc., USA

SOURCE: PCT Int. Appl., 31 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|------------|
| ----- | --- | ----- | ----- | ----- |
| WO 9926661 | A1 | 19990603 | WO 1998-US24412 | 19981116 |
| W: AU, CA, JP | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| US 6197764 | B1 | 20010306 | US 1997-978541 | 19971126 |
| CA 2310850 | AA | 19990603 | CA 1998-2310850 | 19981116 |
| AU 9914115 | A1 | 19990615 | AU 1999-14115 | 19981116 |
| AU 746472 | B2 | 20020502 | | |
| EP 1044023 | A1 | 20001018 | EP 1998-957987 | 19981116 |
| EP 1044023 | B1 | 20050525 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, SE, IE | | | | |
| JP 2001523732 | T2 | 20011127 | JP 2000-521862 | 19981116 |
| AT 296116 | E | 20050615 | AT 1998-957987 | 19981116 |
| ES 2244098 | T3 | 20051201 | ES 1998-957987 | 19981116 |
| PRIORITY APPLN. INFO.: | | | US 1997-978541 | A 19971126 |
| | | | WO 1998-US24412 | W 19981116 |

AB The invention provides compns. that include conjugates of a fatty acid mol., preferably cis-docosahexaenoic acid, and clozapine. The conjugates are useful in treating psychol. disorders such as schizophrenia. Docosahexaenoic acid-clozapine (preparation given) was at least six times longer-acting than clozapine against locomotor behavioral arousal in rats treated with R(-) apomorphine.

IT 120360-10-3, Batelapine maleate

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(pharmaceutical further containing; clozapine conjugate with fatty acid for treating schizophrenia)

RN 120360-10-3 CAPLUS

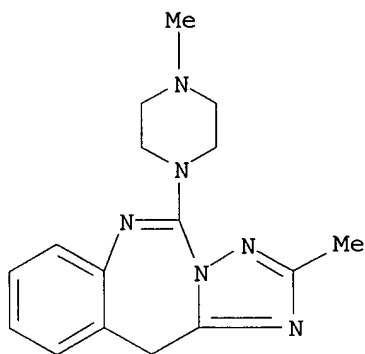
CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 2-methyl-5-(4-methyl-1-piperazinyl)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 95634-82-5

CMF C16 H20 N6

10/019,683

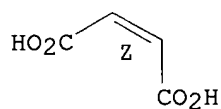


CM 2

CRN 110-16-7

CMF C4 H4 O4

Double bond geometry as shown.



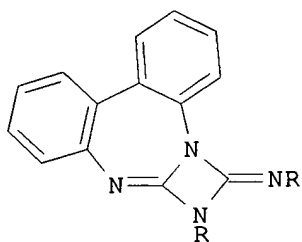
REFERENCE COUNT:

4

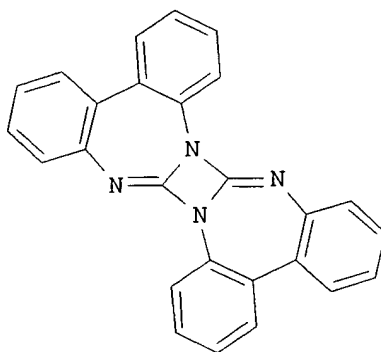
THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

✓
 L14 ANSWER 7 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:46621 CAPLUS
 DOCUMENT NUMBER: 130:209679
 TITLE: Preparation and Intramolecular Cyclization of
 Bis(carbodiimides). Synthesis and X-ray Structure of
 1,3-Diazetidino-2,4-diimine Derivatives
 AUTHOR(S): Alajarin, Mateo; Molina, Pedro; Sanchez-Andrada,
 Pilar; Foces-Foces, M. Concepcion
 CORPORATE SOURCE: Departamento de Quimica Organica Facultad de Quimica,
 Universidad de Murcia, Murcia, E-30071, Spain
 SOURCE: Journal of Organic Chemistry (1999), 64(4), 1121-1130
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 130:209679
 GI



II



IV

AB Aza-Wittig reactions of bis(iminophosphorane) 2-Ph₃P:NC₆H₄C₆H₄N:PPh₃-2 (I), derived from 2,2'-diazidobiphenyl, with aromatic isocyanates provided dibenzo[d,f]-1,3-diazetidino[1,2-a]diazepine derivs. II [R = substituted Ph, 1-naphthyl] in moderate yields. Similar results can be achieved from the reaction of 2,2'-bis(isothiocyanato)biphenyl (III) with aryliminophosphoranes. Treatment of bis(isothiocyanate) III with arylamines and further dehydrosulfurization of the resulting bis(thioureas) leads to seven-membered ring guanidines. (2'-Azido)biphenyl-N'-arylcarbodiimides react with 1 equiv of triphenylphosphine to give zwitterionic compds., which undergo either hydrolytic cleavage to afford guanidines or react with 1 equiv of aromatic isocyanates to provide II. Cross-expts. suggest that the conversion zwitterionic compds. → II takes place through a non-isolable bis(carbodiimide) that undergoes an intramol. [2 + 2] cycloaddn. at the final step. The reaction of bis(iminophosphorane) I with an excess of carbon dioxide leads to a mixture of tricyclic 1,3-diazetidino derivative IV and a 14-membered cyclic bis(carbodiimide), which decomp. by thermal treatment. IV can also be obtained along with seven-membered cyclic urea derivs. from the reaction of bis(iminophosphorane) I with the carbon dioxide source Boc₂O/DMAP system. A comprehensive mechanistic scheme for the aza-Wittig reactions studied is conveniently presented. The mol. and crystal structures of 1-(4-methoxyphenyl)-2-(4-methoxyphenyl)iminodibenzo[d,f]-1,3-diazetidino[1,2-a]diazepine and

[a,c]bis[dibenzo[d,f][1,3]diazepino]-1,3-diazetidene (IV) have been determined by X-ray anal.

IT 194484-24-7P 221011-14-9P 221011-15-0P

221011-16-1P 221011-17-2P 221011-18-3P

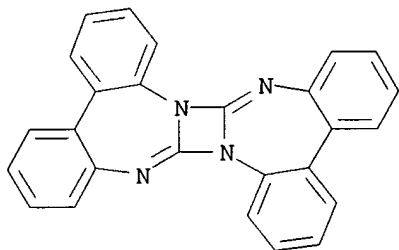
221011-20-7P 221011-37-6P 221011-39-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and intramol. cyclization of bis(carbodiimides))

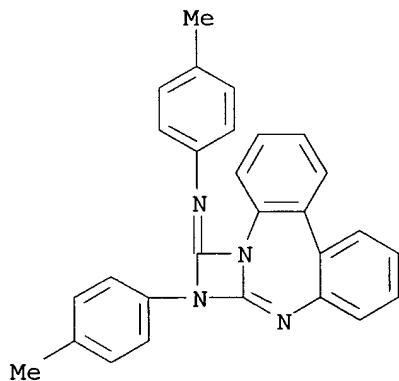
RN 194484-24-7 CAPLUS

CN Tetrabenzo[d,d',f,f'] [1,3]diazeto[1,2-a:3,4-a']bis[1,3]diazepine (9CI)
(CA INDEX NAME)



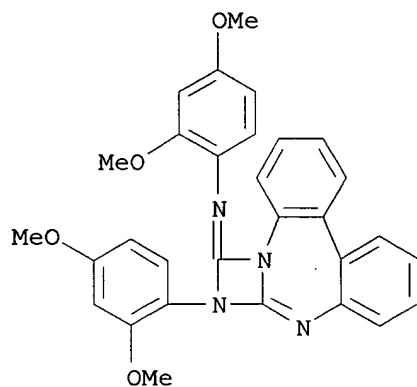
RN 221011-14-9 CAPLUS

CN Benzenamine, 4-methyl-N-[7-(4-methylphenyl)benzo[d][1,3]diazeto[1,2-a][1,3]benzodiazepin-6(7H)-ylidene]- (9CI) (CA INDEX NAME)



RN 221011-15-0 CAPLUS

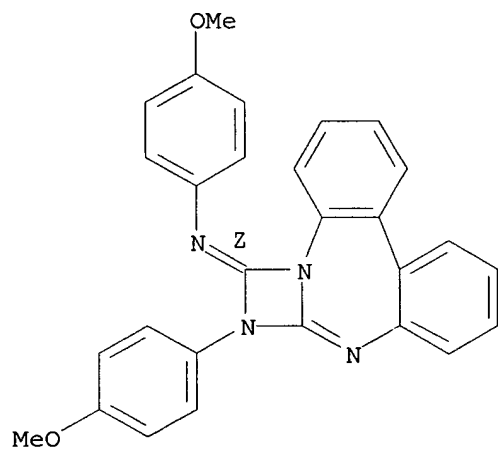
CN Benzenamine, N-[7-(2,4-dimethoxyphenyl)benzo[d][1,3]diazeto[1,2-a][1,3]benzodiazepin-6(7H)-ylidene]-2,4-dimethoxy- (9CI) (CA INDEX NAME)



RN 221011-16-1 CAPLUS

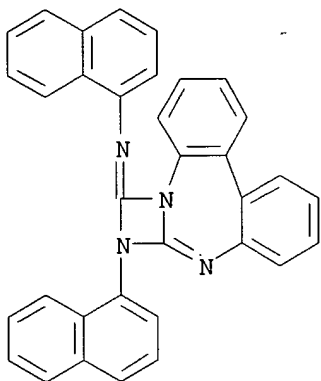
CN Benzenamine, 4-methoxy-N-[7-(4-methoxyphenyl)benzo[d][1,3]diazeto[1,2-a][1,3]benzodiazepin-6(7H)-ylidene]-, [N(Z)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

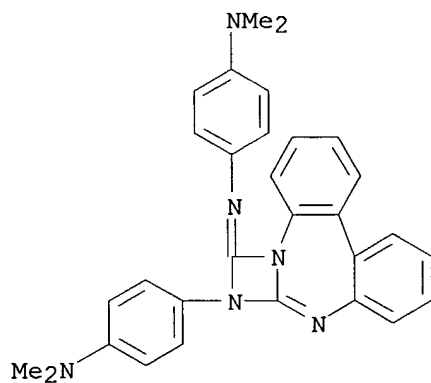


RN 221011-17-2 CAPLUS

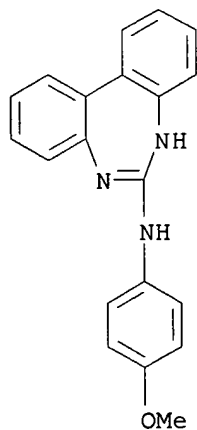
CN 1-Naphthalenamine, N-[7-(1-naphthalenyl)benzo[d][1,3]diazeto[1,2-a][1,3]benzodiazepin-6(7H)-ylidene]- (9CI) (CA INDEX NAME)



RN 221011-18-3 CAPLUS
 CN 1,4-Benzenediamine, N'-[7-[4-(dimethylamino)phenyl]benzo[d][1,3]diazeto[1,2-a][1,3]benzodiazepin-6(7H)-ylidene]-N,N-dimethyl- (9CI) (CA INDEX NAME)



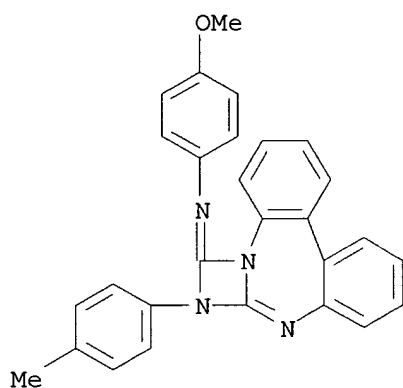
RN 221011-20-7 CAPLUS
 CN 5H-Dibenzo[d,f][1,3]diazepin-6-amine, N-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



10/019,683

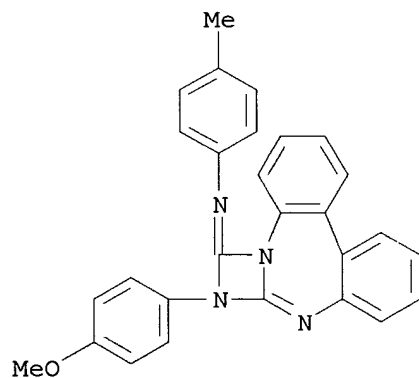
RN 221011-37-6 CAPLUS

CN Benzenamine, 4-methoxy-N-[7-(4-methylphenyl)benzo[d][1,3]diazeto[1,2-a][1,3]benzodiazepin-6(7H)-ylidene]- (9CI) (CA INDEX NAME)



RN 221011-39-8 CAPLUS

CN Benzenamine, N-[7-(4-methoxyphenyl)benzo[d][1,3]diazeto[1,2-a][1,3]benzodiazepin-6(7H)-ylidene]-4-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

37

THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/019,683

114 ANSWER 8 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:288578 CAPLUS

DOCUMENT NUMBER: 128:330412

TITLE: Strategies for the design of biomimetic oxoanion ionophores for ion-selective electrodes

AUTHOR(S): Ball, J. Christopher; Hutchins, Richard S.; Raposo, Cesar; Moran, Joaquin R.; Alajarin, Mateo; Molina, Pedro; Bachas, Leonidas G.

CORPORATE SOURCE: Dep. Chem., Univ. Kentucky, Lexington, KY, 40506-0055, USA

SOURCE: ACS Symposium Series (1998), 690(Polymers in Sensors), 248-256

CODEN: ACSMC8; ISSN: 0097-6156

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Biomimetic ionophores were developed for use in ion-selective electrodes (ISEs). By mimicking the strong interactions between certain biol. mols. and oxoanions, ionophores were designed that demonstrate high selectivity for particular oxoanions. Ionophores based on the guanidinium functional group and a derivatized urea group were prepared ISEs for hydrogen sulfite, salicylate, and ibuprofen based on these ionophores are described.

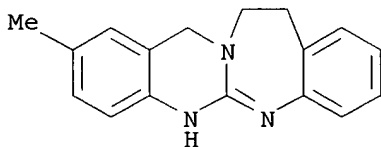
IT 206852-96-2

RL: ARG (Analytical reagent use); DEV (Device component use); ANST (Analytical study); USES (Uses)

(hydrogen sulfite, salicylate, and ibuprofen determination by ion-selective electrodes based on biomimetic ionophores)

RN 206852-96-2 CAPLUS

CN Quinazolino[2,3-b][1,3]benzodiazepine, 5,11,13,14-tetrahydro-9-methyl-, conjugate monoacid (9CI) (CA INDEX NAME)

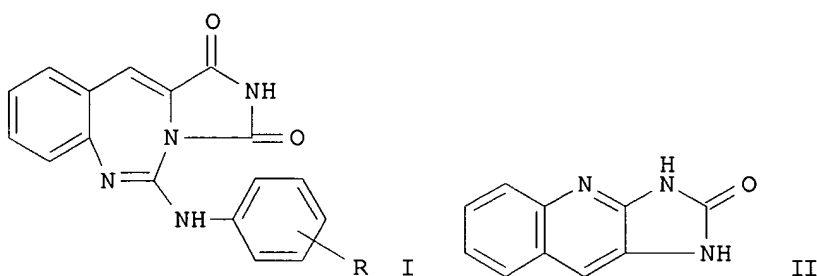


● H⁺

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/019,683

~~114~~ ANSWER 9 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:745383 CAPLUS
DOCUMENT NUMBER: 128:34744
TITLE: Synthesis of imidazo[1,5-c][1,3]benzodiazepines via an
aza-Wittig/carbodiimide-mediated annulation process
AUTHOR(S): Molina, Pedro; Tarraga, Alberto; Curiel, David;
Ramirez de Arellano, Carmen
CORPORATE SOURCE: Dep. Quim. Org., Fac. Quim., Univ. Murcia, Murcia,
E-30071, Spain
SOURCE: Tetrahedron (1997), 53(46), 15895-15902
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

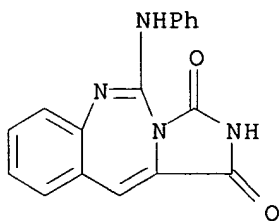


AB The first synthesis of the imidazo[1,5-c][1,3]benzodiazepine ring system, e.g., I (R = H, 4-Me, 2-Me, 4-OMe, 3-OMe, 4-Cl, 4-NO₂), has been carried out by reaction of the iminophosphorane derived from the (Z)-5-(o-azidoarylidene)hydantoin with isocyanates. The isomeric (E)-tributyliminophosphorane undergoes intramol. aza Wittig reaction to give the imidazo[4,5-b]quinolin-2-one ring (II).

IT 199390-42-6P 199390-43-7P 199390-44-8P
199390-45-9P 199390-46-0P 199390-47-1P
199390-48-2P 199390-49-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(imidazo[1,5-c][1,3]benzodiazepines via aza-Wittig/carbodiimide-mediated annulation process)

RN 199390-42-6 CAPLUS

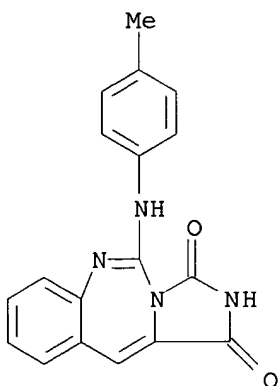
CN 1H-Imidazo[1,5-c][1,3]benzodiazepine-1,3(2H)-dione, 5-(phenylamino)- (9CI)
(CA INDEX NAME)



RN 199390-43-7 CAPLUS

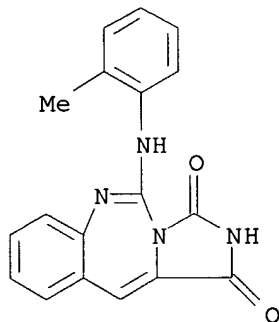
10/019,683

CN 1H-Imidazo[1,5-c][1,3]benzodiazepine-1,3(2H)-dione, 5-[(4-methylphenyl)amino]- (9CI) (CA INDEX NAME)



RN 199390-44-8 CAPLUS

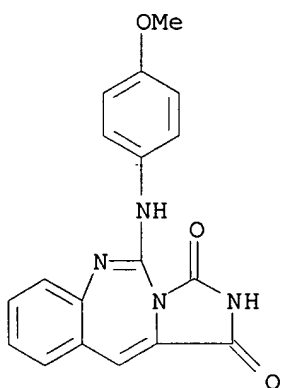
CN 1H-Imidazo[1,5-c][1,3]benzodiazepine-1,3(2H)-dione, 5-[(2-methylphenyl)amino]- (9CI) (CA INDEX NAME)



RN 199390-45-9 CAPLUS

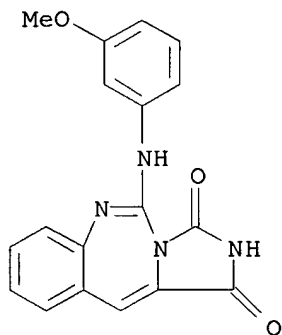
CN 1H-Imidazo[1,5-c][1,3]benzodiazepine-1,3(2H)-dione, 5-[(4-methoxyphenyl)amino]- (9CI) (CA INDEX NAME)

10/019,683



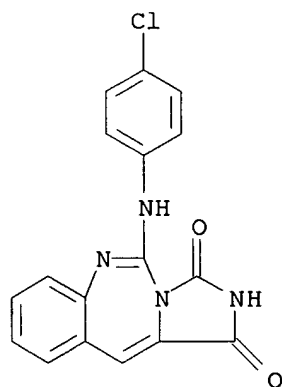
RN 199390-46-0 CAPLUS

CN 1H-Imidazo[1,5-c][1,3]benzodiazepine-1,3(2H)-dione, 5-[(3-methoxyphenyl)amino]- (9CI) (CA INDEX NAME)



RN 199390-47-1 CAPLUS

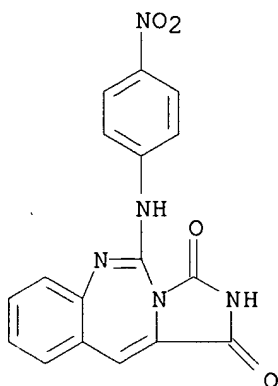
CN 1H-Imidazo[1,5-c][1,3]benzodiazepine-1,3(2H)-dione, 5-[(4-chlorophenyl)amino]- (9CI) (CA INDEX NAME)



RN 199390-48-2 CAPLUS

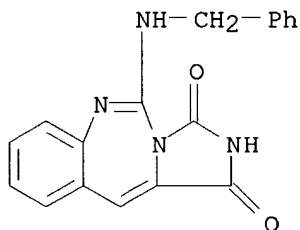
10/019,683

CN 1H-Imidazo[1,5-c][1,3]benzodiazepine-1,3(2H)-dione, 5-[(4-nitrophenyl)amino]- (9CI) (CA INDEX NAME)



RN 199390-49-3 CAPLUS

CN 1H-Imidazo[1,5-c][1,3]benzodiazepine-1,3(2H)-dione, 5-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

18

THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/019,683

~~104~~ ANSWER 10 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:516479 CAPLUS

DOCUMENT NUMBER: 127:190717

TITLE: Studies of cyclic carbodiimides. X-ray crystal structure of [a,c]bis{dibenzo[d,f][1,3]-diazepino}-1,3-diazetidene

AUTHOR(S): Alajarin, Mateo; Molina, Pedro; Sanchez-Andrada, Pilar; Foces-Foces, Concepcion

CORPORATE SOURCE: Dep. Quimica Organica, Fac. Quimica, Univ. Murcia, Murcia, 30071, Spain

SOURCE: Electronic Conference on Heterocyclic Chemistry, [Proceedings], June 24-July 22, 1996 (1997), Meeting Date 1996, No pp. given. Editor(s): Rzepa, Henry S.; Snyder, James P.; Leach, Christopher. Royal Society of Chemistry: Cambridge, UK.
CODEN: 64WTAX

DOCUMENT TYPE: Conference; (computer optical disk)

LANGUAGE: English

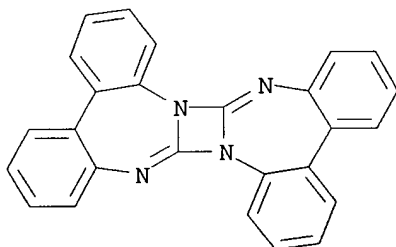
AB A conference report with no refs. The formation and mol. structure of the title compound are discussed; crystal data are not reported.

IT 194484-24-7P

RL: MSC (Miscellaneous); PRP (Properties); SPN (Synthetic preparation);
PREP (Preparation)
(formation and structure of)

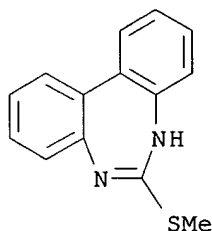
RN 194484-24-7 CAPLUS

CN Tetrabenzo[d,d',f,f'] [1,3]diazeto[1,2-a:3,4-a']bis[1,3]diazepine (9CI)
(CA INDEX NAME)



~~DL4~~ ANSWER 11 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1997:369740 CAPLUS
 DOCUMENT NUMBER: 126:344564
 TITLE: 6-Methylthio-5H-dibenzo[d,f][1,3]diazepine as additive
 in anticorrosive coating with vinyl
 chloride-vinylidene chloride or -vinyl acetate
 copolymer binder and butyl acetate, toluene and
 acetone solvents
 INVENTOR(S): Ambartsumyan, Rafael G.; Shelepin, Oleg E.; Shelepina,
 Viktoriya L.; Bogatyreva, Nuriya K.; Shelepin, Nikolaj
 E.
 PATENT ASSIGNEE(S): Filial "nauchno-Issledovatel'skaya Chast" Ao - Institut
 "rostovskij Promstrojniiproekt", Russia; Tsent
 Naukoemkikh Tekhnologij Mnm "interbios"; Rostovskij
 Gosudarstvennyj Pedagogicheskij Institut
 SOURCE: Russ. From: Izobreteniya 1996, (36), 173.
 CODEN: RUXXE7
 DOCUMENT TYPE: Patent
 LANGUAGE: Russian
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| RU 2070908 | C1 | 19961227 | RU 1994-21723 | 19940608 |
| PRIORITY APPLN. INFO.: | | | RU 1994-21723 | 19940608 |
| AB Title only translated. | | | | |
| IT 2880-29-7 | | | | |
| RL: MOA (Modifier or additive use); USES (Uses) | | | | |
| (methylthiodibenzodiazepine as additive in anticorrosive coating with vinyl chloride-vinylidene chloride or -vinyl acetate copolymer binder and Bu acetate, toluene and acetone solvents) | | | | |
| RN 2880-29-7 CAPLUS | | | | |
| CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(methylthio)- (7CI, 8CI, 9CI) (CA INDEX NAME) | | | | |



10/019,683

114 ANSWER 12 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:515955 CAPLUS

DOCUMENT NUMBER: 122:255375

TITLE: Quantitative determination and pharmacokinetics of a new antipsychotic (CGS 13429A) in human plasma using capillary gas chromatography/mass spectrometry

AUTHOR(S): Carlsen, S.; Hayes, M.; Powell, M. L.

CORPORATE SOURCE: Ciba-Geigy Corp., Ardsley, NY, 10502, USA

SOURCE: Journal of Pharmaceutical and Biomedical Analysis (1995), 13(3), 313-18

CODEN: JPBADA; ISSN: 0731-7085

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A quant. anal. method is described for the determination of a new antipsychotic (CGS 13429A) in human plasma. The method relies on capillary gas chromatog./mass spectrometry in the pos. chemical ionization mode, utilizing ammonia reagent gas. The limit of quantification (LOQ) was 0.1 ng mL⁻¹ and the method was validated over a concentration range of 0.1-50 ng mL⁻¹. The method was used to measure CGS 13429A plasma concns. following the administration of single oral ascending doses ranging from 0.1 to 10 mg in healthy male volunteers. The drug was rapidly absorbed (T_{max} ranged from 1.1 to 3.7 h) and showed a mean terminal elimination half-life of 8.1 h, which was independent of dose. Area-under-the-curve (AUC) along with C_{max} values were proportional to the administered dose.

IT 120360-10-3, CGS 13429A

RL: ANT (Analyte); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process)

(quant. determination and pharmacokinetics of the new antipsychotic CGS

13429A

in human plasma using capillary gas chromatog./mass spectrometry)

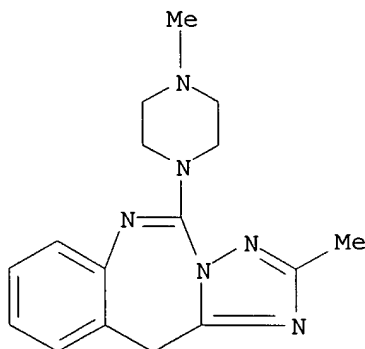
RN 120360-10-3 CAPLUS

CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 2-methyl-5-(4-methyl-1-piperazinyl)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 95634-82-5

CMF C16 H20 N6

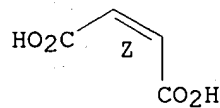


CM 2

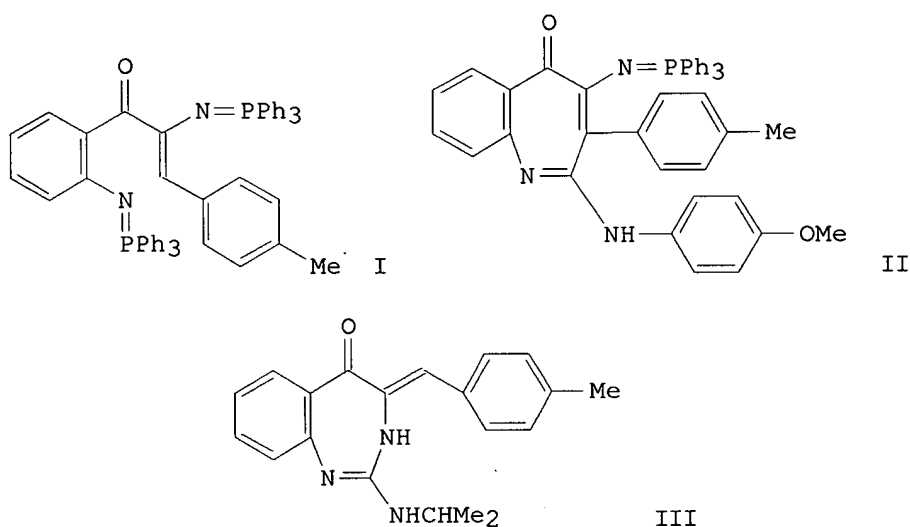
10/019,683

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

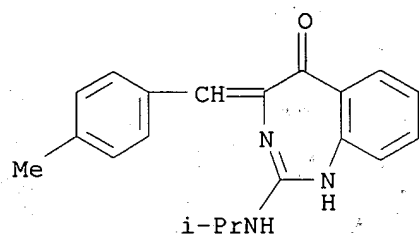


L14 ANSWER 13 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1994:534254 CAPLUS
 DOCUMENT NUMBER: 121:134254
 TITLE: New synthetic applications of vinyliminophosphoranes based on the reactivity of the vinyl side chain
 AUTHOR(S): Molina, Pedro; Aller, Enrique; Lopez-Lazaro, Antonia; Alajarin, Mateo; Lorenzo, Angeles
 CORPORATE SOURCE: Fac. de Quim., Univ. de Murcia, Murcia, E-30071, Spain
 SOURCE: Tetrahedron Letters (1994), 35(22), 3817-20
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 121:134254
 GI



AB New reactions of vinyliminophosphoranes involving either the β -carbon atom of the vinyl side chain as nucleophilic center or the α -carbon as electrophilic center are described. E.g., treating vinyliminophosphorane I with RNCX (R = 4-MeOC₆H₄, X = S, O; R = Me₂CH, X = O) gave cyclized products II or III, resp.
 IT 157034-12-3P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 157034-12-3 CAPLUS
 CN 5H-1,3-Benzodiazepin-5-one, 1,4-dihydro-2-[(1-methylethyl)amino]-4-[(4-methylphenyl)methylene]- (9CI) (CA INDEX NAME)

10/019,683



14 ANSWER 14 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:234023 CAPLUS

DOCUMENT NUMBER: 118:234023

TITLE: Synthetic applications of bis(iminophosphoranes).
One-pot preparation of rigid bicyclic guanidines

AUTHOR(S): Molina, Pedro; Alajarin, Mateo; Vidal, Angel

CORPORATE SOURCE: Fac. Quim., Univ. Murcia, Murcia, E-30071, Spain

SOURCE: Journal of Organic Chemistry (1993), 58(7), 1687-95

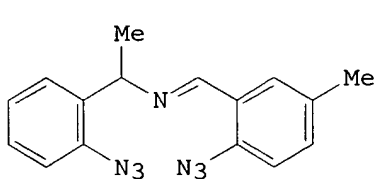
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

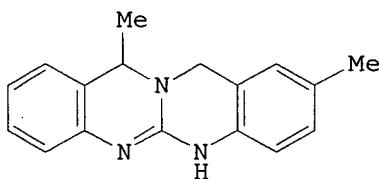
LANGUAGE: English

OTHER SOURCE(S): CASREACT 118:234023

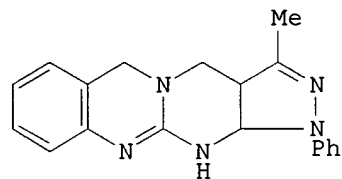
GI



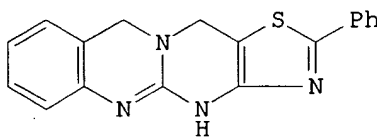
I



II



III



IV

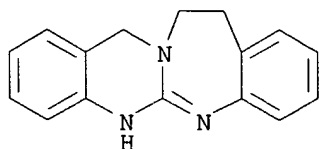
AB A one-pot synthesis of [6+6], [6+7], and [6+8] bicyclic guanidines based on a new method of dihydropyrimido annelation, which involves reaction of bis(iminophosphoranes) with aryl isocyanates or isothiocyanates is described. The method is also applicable for the preparation of chiral bicyclic guanidines. Condensation of 2-azido-5-methylbenzaldehyde with 1-(2-azidophenyl)ethylamine gave N-(2-azido-5-methylbenzylidene)- α -methyl-2-azidobenzylamine (I). Treatment of I with triphenylphosphine followed by treatment with sodium borohydride and 4-methylphenyl isocyanate gave the bicyclic guanidine II. Other bicyclic guanidines, such as III or IV, were prepared by a similar route.

IT 146954-34-9P 146954-35-0P 146954-36-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from bis(iminophosphorane) derivative)

RN 146954-34-9 CAPLUS

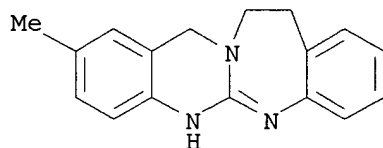
CN Quinazolino[2,3-b][1,3]benzodiazepine, 5,11,13,14-tetrahydro- (9CI) (CA INDEX NAME)



10/019,683

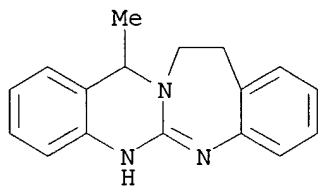
RN 146954-35-0 CAPLUS

CN Quinazolino[2,3-b][1,3]benzodiazepine, 5,11,13,14-tetrahydro-9-methyl-
(9CI) (CA INDEX NAME)



RN 146954-36-1 CAPLUS

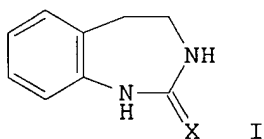
CN Quinazolino[2,3-b][1,3]benzodiazepine, 5,11,13,14-tetrahydro-11-methyl-
(9CI) (CA INDEX NAME)



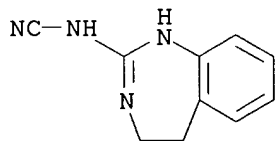
L14 ANSWER 15 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:448620 CAPLUS
 DOCUMENT NUMBER: 117:48620
 TITLE: Preparation of 2-substituted hydrogenated
 1,3-benzodiazepines
 INVENTOR(S): Spindler, Juergen; Kempter, Gerhard; Peseke, Klaus;
 Kleinpeter, Erich
 PATENT ASSIGNEE(S): Paedagogische Hochschule Potsdam, Germany
 SOURCE: Ger. (East), 4 pp.
 CODEN: GEXXA8
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------------------|----------|-----------------|----------|
| ----- | ---- | ----- | ----- | ----- |
| DD 294714 | A5 | 19911010 | DD 1990-341027 | 19900528 |
| PRIORITY APPLN. INFO.: | | | DD 1990-341027 | 19900528 |
| OTHER SOURCE(S): | CASREACT 117:48620 | | | |
| GI | | | | |

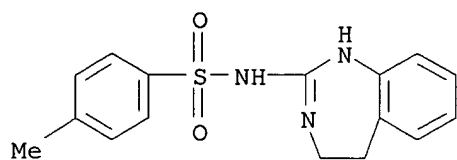


AB Title compds. I [X = C(CN)₂, C(CN)CO₂Et, NCN, NSO₂C₆H₄Me-4] were obtained
 in 43-69% yield by treating 2-H₂NC₆H₄CH₂CH₂NH₂ with X:C(SMe)₂.
 IT 137155-02-3P 137155-06-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 137155-02-3 CAPLUS
 CN Cyanamide, (4,5-dihydro-1H-1,3-benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)



RN 137155-06-7 CAPLUS
 CN Benzenesulfonamide, N-(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)-4-methyl-
 (9CI) (CA INDEX NAME)

10/019,683



L14 ANSWER 16 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:632171 CAPLUS

DOCUMENT NUMBER: 115:232171

TITLE: Substituted quinazolines and benzodiazepines from 1,3- and 1,4-diamines

AUTHOR(S): Spindler, Juergen

CORPORATE SOURCE: Inst. Org. Chem., Univ. Potsdam, Potsdam, O-1571, Germany

SOURCE: Chemiker-Zeitung (1991), 115(7-8), 224-5

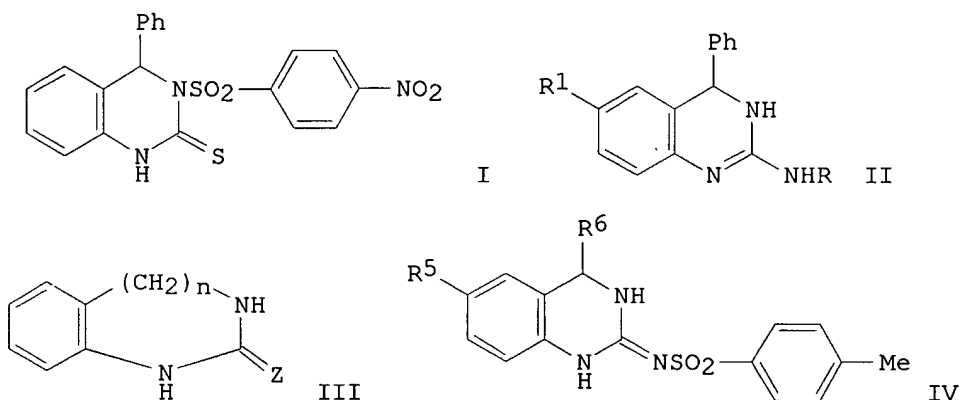
CODEN: CMKZAT; ISSN: 0009-2894

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 115:232171

GI



AB Title compds. I, II [$R = N:C(CO_2Me)CH_2CO_2Me$, $R_1 = H, Cl, Me$; $R = NHSO_2C_6H_2R_2-3-R_3-4-R_4-5$, $R_1 = H, Cl$, $R_2 = R_4 = H$, $R_3 = Me, Br, NO_2$], III [$n = 1, 2$, $Z = C(CN)_2, C(CN)CO_2Et, NCN, NSO_2C_6H_4Me-p$], and IV ($R_5 = H$, $R_6 = Me, Ph$; $R_5 = Cl$, $R_6 = Ph$) were prepared by the following methods. Cyclization of 2-(4-O₂NC₆H₄SO₂NHCHPh)C₆H₄NH₂ with CS₂ gave I. Reactions of II ($R = NH_2$) with MeO₂C-C.tplbond.C-CO₂Me or 3-R₂-4-R₃-5-R₄C₆H₂SO₂Cl gave II [$R = N:C(CO_2Me)CH_2CO_2Me$; $NHSO_2C_6H_2R_2-3-R_3-4-R_4-5$, resp.]. Cyclocondensation of 2-(NH₂(CH₂)_n)C₆H₄NH₂ with (MeS)₂C:Z gave III. IV was prepared from p-MeC₆H₄SO₂N:C(SMe)₂ and 2-R₆CH(NH₂)-3-R₅C₆H₃NH₂.

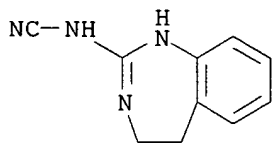
IT 137155-02-3P 137155-06-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, via cyclocondensation of (aminoethyl)aniline with bis(methylthio)methylene compds.)

RN 137155-02-3 CAPLUS

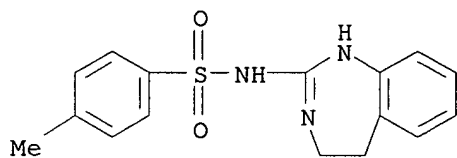
CN Cyanamide, (4,5-dihydro-1H-1,3-benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)



10/019,683

RN 137155-06-7 CAPLUS

CN Benzenesulfonamide, N-(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)-4-methyl-
(9CI) (CA INDEX NAME)



114 ANSWER 17 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:622717 CAPLUS

DOCUMENT NUMBER: 115:222717

TITLE: Determination of in vivo hepatic extraction ratio from in vitro metabolism by rat hepatocytes

AUTHOR(S): Singh, Kuldeep; Tripp, Spencer L.; Dunton, Alan W.; Douglas, Frank L.; Rakhit, Ashok

CORPORATE SOURCE: Res. Dep., Ciba-Geigy Corp., Summit, NJ, 07901, USA

SOURCE: Drug Metabolism and Disposition (1991), 19(5), 990-6

CODEN: DMDSAI; ISSN: 0090-9556

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Using isolated rat hepatocytes, the in vitro intrinsic hepatic clearance of three drugs, namely, antipyrine (AP), propranolol (P), and CGS 13429 was determined. The hepatic extraction ratios of AP, P, and CGS 13429 were then calculated to be 0.10, 0.90, and 0.88, resp. To determine the in vivo hepatic extraction ratio in the rat, AP, P, or CGS 13429 was infused sep. at a rate of 40, 20, and 20 µg/min.kg, via jugular and hepatic portal veins. The steady state plasma levels of AP, P, and CGS 13429 were 5.30 µg/mL, 608 and 380 ng/mL after jugular vein (i.v.) infusions, and 4.96 µg/mL, 162, and 146 ng/mL after hepatic portal vein (hvp) infusions, resp. The blood to plasma ratios of AP, P, and CGS 13429 were 1.0, 0.78, and 1.0, resp. The in vivo hepatic extraction ratio, calculated as $(C_{ss,iv} - C_{ss,hpv})/C_{ss,iv}$ from

steady state blood levels following i.v. and hvp infusions for AP, P, and CGS 13429, were 0.065, 0.73, and 0.61, resp. These results suggest that in vitro metabolism studies by hepatocytes may have potential application, during drug discovery, to distinguish drugs of low and high metabolic hepatic extraction ratio in vivo.

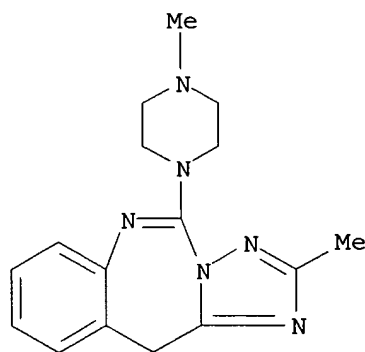
IT 95634-82-5, CGS 13429

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(metabolism of, by hepatocytes, liver extraction ratio determination from)

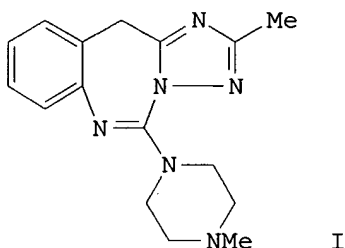
RN 95634-82-5 CAPLUS

CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 2-methyl-5-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

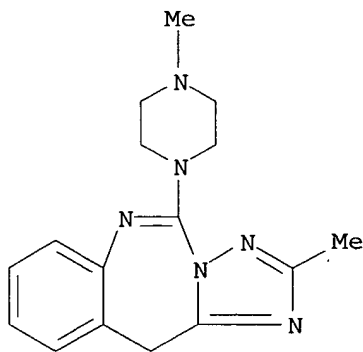


~~114~~ ANSWER 18 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

~~114~~ ACCESSION NUMBER: 1990:95 CAPLUS
 DOCUMENT NUMBER: 112:95
 TITLE: High-performance liquid chromatographic method for a
 clozapine analog, CGS 13429, and its N-oxide and
 demethyl metabolites
 AUTHOR(S): Chovan, James P.; Vermeulen, Jeannette D.
 CORPORATE SOURCE: Pharm. Div., Ciba-Geigy Corp., Ardsley, NY, 10502, USA
 SOURCE: Journal of Chromatography (1989), 494, 413-19
 CODEN: JOCRAM; ISSN: 0021-9673
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

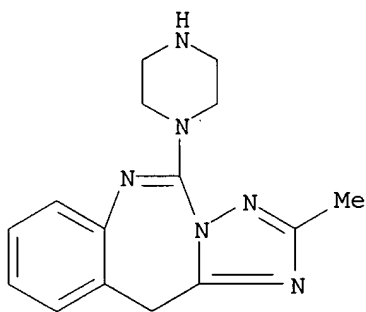


AB An HPLC method for preclin. pharmacokinetic and bioavailability studies to
 quantify a clozapine analog, CGS 13429 (I), and its N-dimethyl and N-oxide
 metabolite is described. The limit of detection was 40 ng/mL for 200
 µL of rat or dog plasma for all 3 compds. The clozapine analog CGS
 11760 was used as internal standard
 IT 95634-82-5, CGS 13429 124027-45-8 124027-46-9
 RL: ANT (Analyte); ANST (Analytical study)
 (determination of, in blood by HPLC)
 RN 95634-82-5 CAPLUS
 CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 2-methyl-5-(4-methyl-1-
 piperazinyl)- (9CI) (CA INDEX NAME)



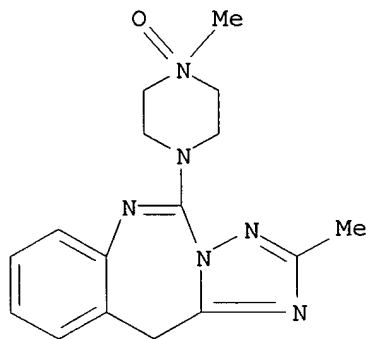
RN 124027-45-8 CAPLUS
 CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 2-methyl-5-(1-piperazinyl)-
 (9CI) (CA INDEX NAME)

10/019,683



RN 124027-46-9 CAPLUS

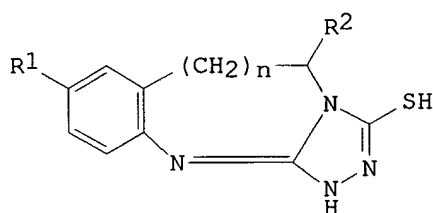
CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 2-methyl-5-(4-methyl-4-oxido-1-piperazinyl)- (9CI) (CA INDEX NAME)



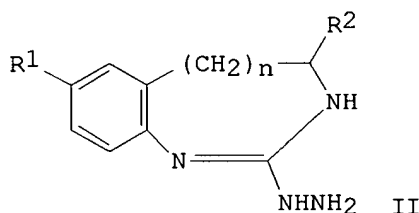
L14 ANSWER 19 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1989:594805 CAPLUS
 DOCUMENT NUMBER: 111:194805
 TITLE: Preparation of 1,2,4-triazolobenzo-1,3-diazacycloheptanes and -octanes
 INVENTOR(S): Spindler, Juergen; Kempster, Gerhard; Schroeder, Christine
 PATENT ASSIGNEE(S): Paedagogische Hochschule Potsdam, Ger. Dem. Rep.
 SOURCE: Ger. (East), 3 pp.
 CODEN: GEXXA8
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|------------|-----------------|----------|
| DD 265897 | A1 | 19890315 | DD 1987-308779 | 19870727 |
| PRIORITY APPLN. INFO.: | | | DD 1987-308779 | 19870727 |
| OTHER SOURCE(S): | MARPAT | 111:194805 | | |

GI

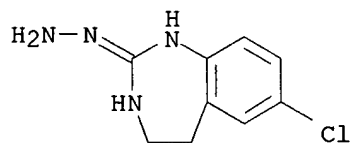


I



II

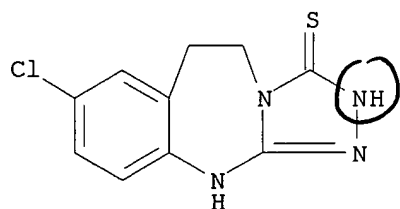
AB The title compds. (I; R1 = H, Cl; R2 = H, Ph; n = 1,2) were prepared by cyclocondensation of hydrazino derivative II with CS2. Thus, II (R1 = Cl, R1 = H, n = 1) was refluxed 6 h with a 5-fold excess of CS2 in MeOH-EtOH containing KOH to give 73% I (R1, R2, n as above).
 IT 120075-93-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclocondensation of, with carbon disulfide)
 RN 120075-93-6 CAPLUS
 CN 2H-1,3-Benzodiazepin-2-one, 7-chloro-1,3,4,5-tetrahydro-, hydrazone (9CI)
 (CA INDEX NAME)



IT 123403-58-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 123403-58-7 CAPLUS
 CN 3H-1,2,4-Triazolo[3,4-b][1,3]benzodiazepine-3-thione, 8-chloro-1,2,5,6-

10/019,683

tetrahydro- (9CI) (CA INDEX NAME)



L14 ANSWER 20 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:173269 CAPLUS

DOCUMENT NUMBER: 110:173269

TITLE: Dihydroquinazolines, dihydrobenzodiazepines and tetrahydrobenzodiazocines as intermediates for bioactive compounds

INVENTOR(S): Spindler, Juergen; Kempster, Gerhard; Schroeder, Christine; Jumar, Alfred

PATENT ASSIGNEE(S): VEB Fahlberg-List, Ger. Dem. Rep.

SOURCE: Ger. (East), 4 pp.

CODEN: GEXXA8

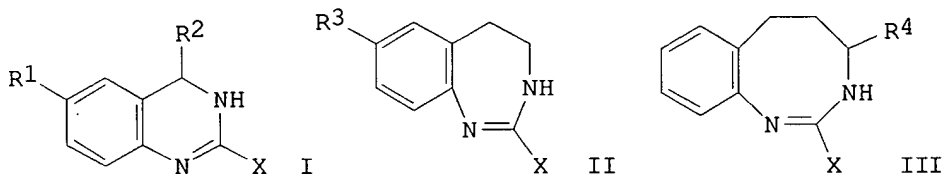
DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|-------------------|----------|-----------------|----------|
| DD 258810 | A1 | 19880803 | DD 1987-300969 | 19870320 |
| PRIORITY APPLN. INFO.: | | | DD 1987-300969 | 19870320 |
| OTHER SOURCE(S): | MARPAT 110:173269 | | | |
| GI | | | | |

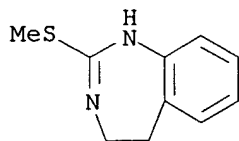


AB The title compds. (I, II, and III; R¹, R³ = halo; R², R⁴ = alkyl, aryl; X = NHNH₂), useful as intermediates for potentially bioactive compds., were prepared from the hydroiodide salts of the corresponding compds. I, II, and III (X = SMe) by reaction with N₂H₄. 4-Methyl-2-methylthio-3,4-dihydroquinazoline.HI was refluxed 45 min in 25% aqueous N₂H₄ to give 85% 2-hydrazino-4-methyl-3,4-dihydroquinazoline.

IT 52063-46-4 97844-45-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrazinolysis of)

RN 52063-46-4 CAPLUS

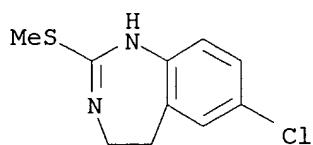
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(methylthio)-, monohydriodide (9CI)
(CA INDEX NAME)

● HI

10/019,683

RN 97844-45-6 CAPLUS

CN 1H-1,3-Benzodiazepine, 7-chloro-4,5-dihydro-2-(methylthio)-,
monohydriodide (9CI) (CA INDEX NAME)



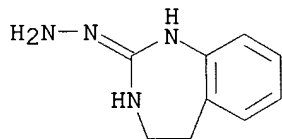
● HI

IT 120075-92-5P 120075-93-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for bioactive compds.)

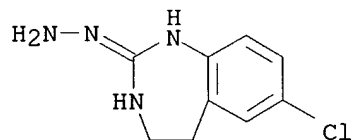
RN 120075-92-5 CAPLUS

CN 2H-1,3-Benzodiazepin-2-one, 1,3,4,5-tetrahydro-, hydrazone (9CI) (CA
INDEX NAME)



RN 120075-93-6 CAPLUS

CN 2H-1,3-Benzodiazepin-2-one, 7-chloro-1,3,4,5-tetrahydro-, hydrazone (9CI)
(CA INDEX NAME)



L14 ANSWER 21 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:493053 CAPLUS

DOCUMENT NUMBER: 109:93053

TITLE: Preparation of 2-heterocyclyl-3,4-dihydroquinazolines,
-4,5-dihydro-3H-1,3-benzodiazepines, and
-3,4,5,6-tetrahydro-1,3-benzodiazocines

INVENTOR(S): Spindler, Juergen; Kempster, Gerhard; Kuehne, Sabine

PATENT ASSIGNEE(S): VEB Fahlberg-List, Ger. Dem. Rep.

SOURCE: Ger. (East), 5 pp.

CODEN: GEXXA8

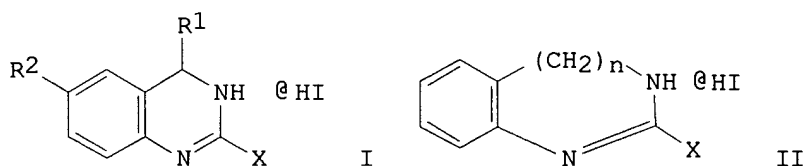
DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------------------|----------|-----------------|----------|
| DD 251977 | A1 | 19871202 | DD 1986-293593 | 19860812 |
| PRIORITY APPLN. INFO.: | | | DD 1986-293593 | 19860812 |
| OTHER SOURCE(S): | CASREACT 109:93053 | | | |
| GI | | | | |

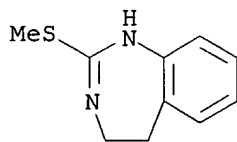


AB The title compds. (I and II; X = heterocyclic secondary amino, e.g., morpholino, pyrrolidino; R¹, R² = alkyl, aryl, halo; n = 2, 3) were prepared as intermediates for bioactive compds. 2-Methylthio-3,4-dihydroquinazoline-HI, morpholine, and HI were refluxed 10 h in EtOH to give 76% 2-morpholino-3,4-dihydroquinazoline-HI.

IT 52063-46-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(amination of, by morpholine)

RN 52063-46-4 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(methylthio)-, monohydriodide (9CI)
(CA INDEX NAME)

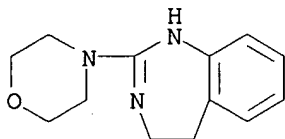
● HI

IT 115787-40-1P 115787-41-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

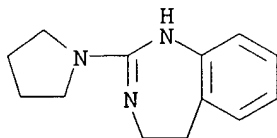
10/019,683

(preparation of)
RN 115787-40-1 CAPLUS
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(4-morpholinyl)-, monohydriodide
(9CI) (CA INDEX NAME)



● HI

RN 115787-41-2 CAPLUS
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(1-pyrrolidinyl)-, monohydriodide
(9CI) (CA INDEX NAME)



● HI

L14 ANSWER 22 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:493052 CAPLUS

DOCUMENT NUMBER: 109:93052

TITLE: Preparation of 2-methylthioquinazolines,
-benzodiazepines, and -benzodiazocines as
intermediates for biological active compounds

INVENTOR(S): Spindler, Juergen; Kempster, Gerhard; Heinemann,
Birgit; Jumar, Alfred

PATENT ASSIGNEE(S): VEB Fahlberg-List, Ger. Dem. Rep.

SOURCE: Ger. (East), 4 pp.

CODEN: GEXXA8

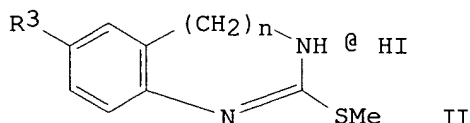
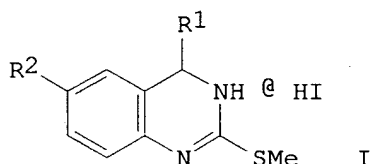
DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------------|------|----------|-----------------|----------|
| DD 251974 | A1 | 19871202 | DD 1986-293592 | 19860812 |
| PRIORITY APPLN. INFO.: GI | | | DD 1986-293592 | 19860812 |



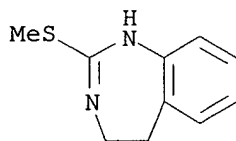
AB The title compds. (I and II; R1,R2,R3 = alkyl, aryl, halo), were prepared by cyclocondensation of CS2 with the corresponding diamines followed by treatment of the unisolated thione intermediates with MeI. 2-Aminobenzylamine and CS2 were kept in EtOH at room temperature for 1 day and then refluxed 3 h to give 55% 3,4-dihydro-1H-quinazoline-2-thione, which was refluxed with MeI in MeOH/EtOH to give 51% 2-methylthio-3,4-dihydroquinazoline-HI (based on starting amine).

IT 52063-46-4P 115724-99-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 52063-46-4 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(methylthio)-, monohydriodide (9CI)
(CA INDEX NAME)

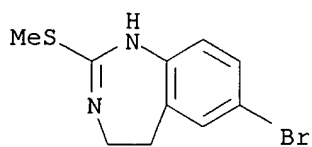


● HI

10/019,683

RN 115724-99-7 CAPLUS

CN 1H-1,3-Benzodiazepine, 7-bromo-4,5-dihydro-2-(methylthio)-, monohydriodide
(9CI) (CA INDEX NAME)



● HI

L14 ANSWER 23 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:598289 CAPLUS

DOCUMENT NUMBER: 107:198289

TITLE: Reaction of cyclic N,N'-disubstituted thioureas with carbonyl activated dielectrophiles

AUTHOR(S): Spindler, Juergen; Kempster, Gerhard

CORPORATE SOURCE: Sekt. Chem./Biol., Paedagog. Hochsch. "Karl Liebknecht", Potsdam, DDR-1500, Ger. Dem. Rep.

SOURCE: Zeitschrift fuer Chemie (1987), 27(1), 36-7

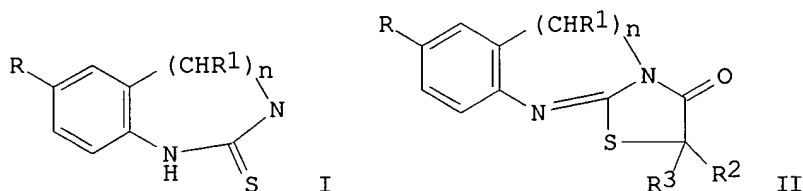
CODEN: ZECEAL; ISSN: 0044-2402

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 107:198289

GI

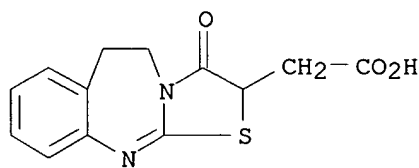


AB The reaction of cyclic thioureas I (R = H, Cl; R₁ = Me, Ph; n = 1; R = R₁ = H; n = 2, 3) with BrCH₂CO₂Et, MeO₂CC.tplbond.CCO₂Me and maleic anhydride gave condensed thiazolones II (R₂ = H, CH₂CO₂H, R₃ = H; R₂R₃ = methoxycarbonylmethylene).

IT 111039-32-8P 111039-33-9P

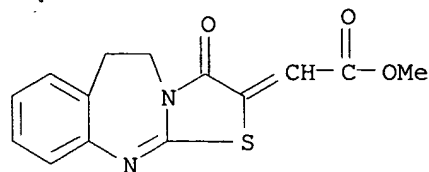
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 111039-32-8 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine-2-acetic acid, 2,3,5,6-tetrahydro-3-oxo-
(9CI) (CA INDEX NAME)

RN 111039-33-9 CAPLUS

CN Acetic acid, (5,6-dihydro-3-oxothiazolo[2,3-b][1,3]benzodiazepin-2(3H)-ylidene)-, methyl ester (9CI) (CA INDEX NAME)



~~DI 4~~ ANSWER 24 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1986:19542 CAPLUS

DOCUMENT NUMBER: 104:19542

TITLE: Photochemical formation of methylenecyclopropane analogs. 11. Photochemical elimination of nitrogen from phenyl-substituted 1,4-dihydro-5-imino-5H-tetrazoles. Products of phenyl-substituted tris(imino)methane diradicals

AUTHOR(S): Quast, Helmut; Fuss, Andreas; Nahr, Uwe

CORPORATE SOURCE: Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, D-8700, Fed. Rep. Ger.

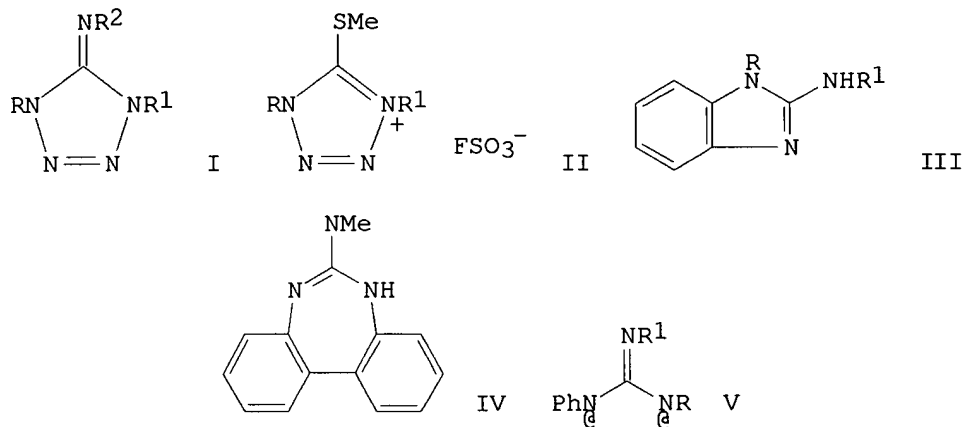
SOURCE: Chemische Berichte (1985), 118(6), 2164-85
CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 104:19542

GI



AB The title iminotriazoles (I; R = R1 = Me, R2 = Ph; R = Ph, R1 = Me, R2 = Me, Ph; R = R1 = Ph, R2 = Me), prepared by reaction of (methylthio)thiazolium compds. II with R2NH2, underwent photolysis with elimination of mol. N to give chiefly 2-aminobenzimidazoles III plus PhNHC(:NR)NHR1 and aminodibenzodiazepine IV (where 2 of R-R2 = Ph). Photolysis of I (R = Ph, R1 = Me, R2 = CD3, C6D5) led to scrambling of the D among the possible positions giving, e.g., equal amts. of II (R = CD3, R1 = Me; R = Me, R1 = CD3), demonstrating the equivalence of N atoms N-1, N-4, and the exocyclic N with respect to product formation. Tris(imino)methane diradicals V are postulated as intermediates in the photochem. process.

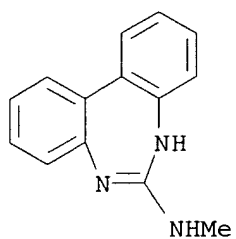
IT 2849-05-0P 97990-14-2P

RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in photolysis of iminotetrazole derivative)

RN 2849-05-0 CAPLUS

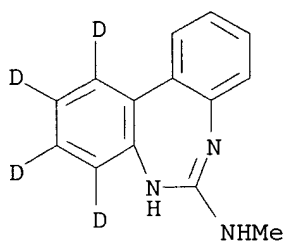
CN 5H-Dibenzo[d,f][1,3]diazepin-6-amine, N-methyl- (9CI) (CA INDEX NAME)

10/019,683



RN 97990-14-2 CAPLUS

CN 5H-Dibenzo[d, f][1, 3]diazepin-1, 2, 3, 4-d4-6-amine, N-methyl- (9CI) (CA
INDEX NAME)



L14 ANSWER 25 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:505012 CAPLUS

DOCUMENT NUMBER: 103:105012

TITLE: Imidazo acid and pyrimido [2,1-b]-1,3-benzodiazepines
and their use as antidepressants

INVENTOR(S): Ferrand, Gerard; Depin, Jean Claude

PATENT ASSIGNEE(S): LIPHA, Lyonnaise Industrielle Pharmaceutique, Fr.

SOURCE: Fr. Demande, 23 pp.

CODEN: FRXXBL

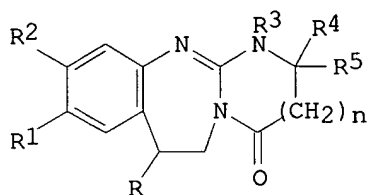
DOCUMENT TYPE: Patent

LANGUAGE: French

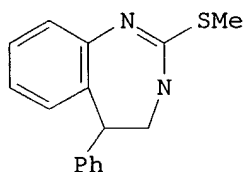
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|--|-----------------|----------|
| FR 2550199 | A1 | 19850208 | FR 1983-12703 | 19830802 |
| FR 2550199 | B1 | 19851129 | | |
| PRIORITY APPLN. INFO.: | | | FR 1983-12703 | 19830802 |
| OTHER SOURCE(S): | | CASREACT 103:105012; MARPAT 103:105012 | | |
| GI | | | | |



I



II

AB Title compds. I ($n = 0, 1$; $R = H, Me, Ph, \text{halo-}, \text{alkyl-}, \text{or alkoxyphenyl}$; $R_1 = H, \text{halo}, \text{alkyl}, \text{alkoxy}$; $R_2 = H, OMe$; $R_3 = H, \text{alkyl}, \text{carbalkoxy}$; $R_4 = H, Me, Ph$; $R_5 = H, Me$), which were prepared, exhibited antidepressant activity. A mixture of benzodiazepine derivative II and $H_2NCH_2CO_2Et$ in MeCN

was

stirred at room temperature to give I ($n = 0, R = Ph, R_1 = R_2 = R_3 = R_4 = R_5 = H$).

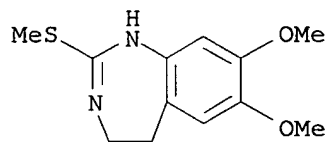
IT 37852-20-3 97866-87-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(a cyclic condensation of, with glycinate ester)

RN 37852-20-3 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-7,8-dimethoxy-2-(methylthio)-,
monohydriodide (9CI) (CA INDEX NAME)

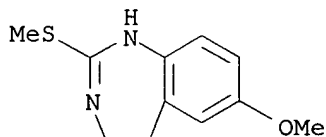


● HI

10/019,683

RN 97866-87-0 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-7-methoxy-2-(methylthio)-,
monohydriodide (9CI) (CA INDEX NAME)



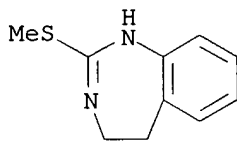
● HI

IT 52063-46-4 90141-77-8 97844-45-6
97844-59-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclic condensation of, with amino acid esters)

RN 52063-46-4 CAPLUS

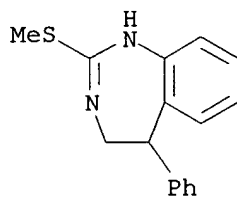
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(methylthio)-, monohydriodide (9CI)
(CA INDEX NAME)



● HI

RN 90141-77-8 CAPLUS

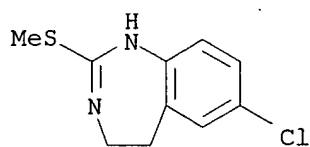
CN 3H-1,3-Benzodiazepine, 4,5-dihydro-2-(methylthio)-5-phenyl-,
monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 97844-45-6 CAPLUS

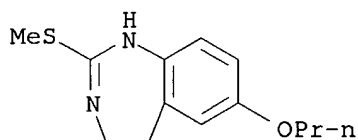
CN 1H-1,3-Benzodiazepine, 7-chloro-4,5-dihydro-2-(methylthio)-,
monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 97844-59-2 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(methylthio)-7-propoxy-,
monohydriodide (9CI) (CA INDEX NAME)



● HI

IT 90156-43-7 90156-45-9 94568-07-7

94568-09-9 94568-11-3 94568-13-5

97844-62-7 97844-94-5 97844-97-8

97845-00-6 97845-03-9 97845-08-4

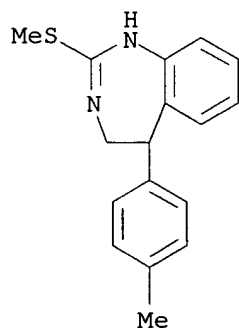
97845-11-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(cyclic condensation of, with glycinate ester)

RN 90156-43-7 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-(4-methylphenyl)-2-(methylthio)-,
monohydriodide (9CI) (CA INDEX NAME)

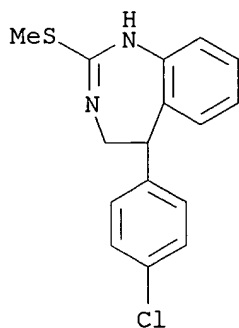


● HI

10/019,683

RN 90156-45-9 CAPLUS

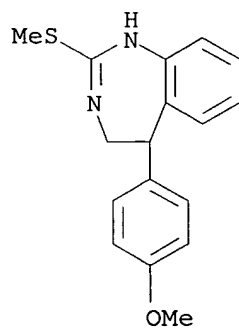
CN 1H-1,3-Benzodiazepine, 5-(4-chlorophenyl)-4,5-dihydro-2-(methylthio)-,
monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 94568-07-7 CAPLUS

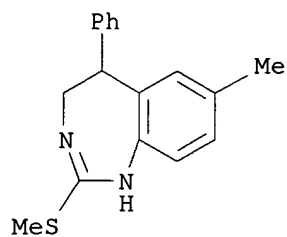
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-(4-methoxyphenyl)-2-(methylthio)-,
monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 94568-09-9 CAPLUS

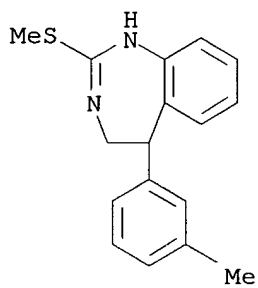
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-7-methyl-2-(methylthio)-5-phenyl-,
monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 94568-11-3 CAPLUS

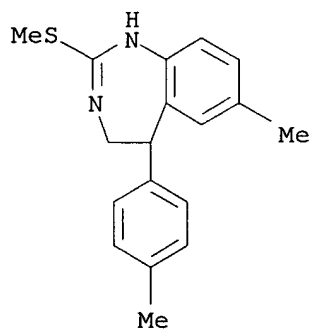
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-(3-methylphenyl)-2-(methylthio)-, monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 94568-13-5 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-7-methyl-5-(4-methylphenyl)-2-(methylthio)-, monohydriodide (9CI) (CA INDEX NAME)

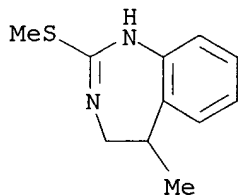


● HI

10/019,683

RN 97844-62-7 CAPLUS

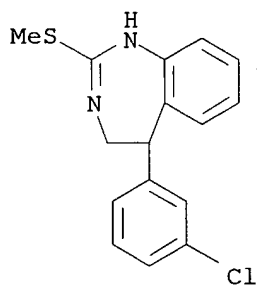
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-methyl-2-(methylthio)-,
monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 97844-94-5 CAPLUS

CN 1H-1,3-Benzodiazepine, 5-(3-chlorophenyl)-4,5-dihydro-2-(methylthio)-,
monohydriodide (9CI) (CA INDEX NAME)

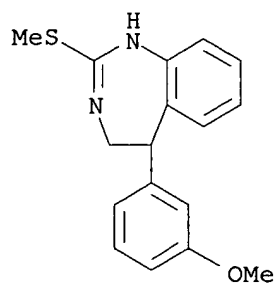


● HI

RN 97844-97-8 CAPLUS

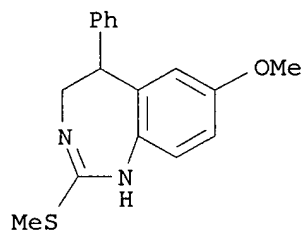
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-(3-methoxyphenyl)-2-(methylthio)-,
monohydriodide (9CI) (CA INDEX NAME)

10/019,683



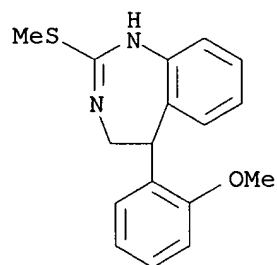
● HI

RN 97845-00-6 CAPLUS
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-7-methoxy-2-(methylthio)-5-phenyl-,
monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 97845-03-9 CAPLUS
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-(2-methoxyphenyl)-2-(methylthio)-,
monohydriodide (9CI) (CA INDEX NAME)

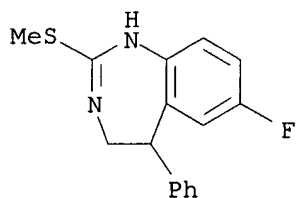


● HI

RN 97845-08-4 CAPLUS

10/019,683

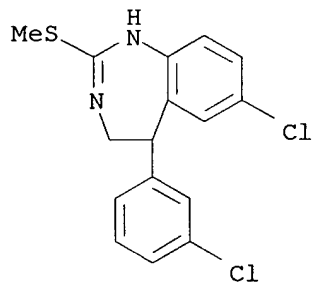
CN 1H-1,3-Benzodiazepine, 7-fluoro-4,5-dihydro-2-(methylthio)-5-phenyl-,
monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 97845-11-9 CAPLUS

CN 1H-1,3-Benzodiazepine, 7-chloro-5-(3-chlorophenyl)-4,5-dihydro-2-(methylthio)-, monohydriodide (9CI) (CA INDEX NAME)



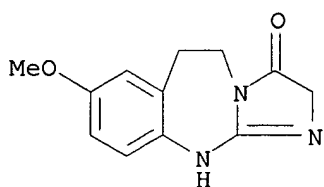
● HI

IT 97844-55-8P 97844-58-1P 97844-84-3P
97844-93-4P 97844-96-7P 97845-07-3P
97845-10-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and antidepressant activity of)

RN 97844-55-8 CAPLUS

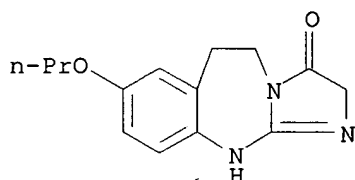
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-8-methoxy-, monohydrochloride (9CI) (CA INDEX NAME)



ex. 28

● HCl

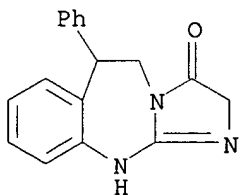
RN 97844-58-1 CAPLUS
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-8-propoxy-,
monohydrochloride (9CI) (CA INDEX NAME)



ex. 30

● HCl

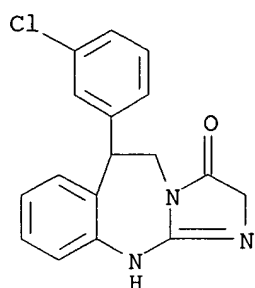
RN 97844-84-3 CAPLUS
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-6-phenyl-,
monohydrochloride (9CI) (CA INDEX NAME)



ex 1

● HCl

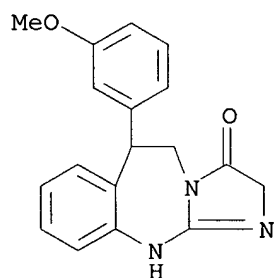
RN 97844-93-4 CAPLUS
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 6-(3-chlorophenyl)-1,2,5,6-
tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)



Ex. 7

● HCl

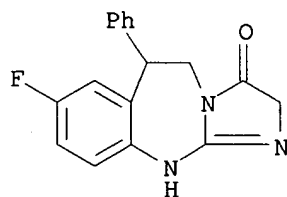
RN 97844-96-7 CAPLUS
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-6-(3-methoxyphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



Ex. 9

● HCl

RN 97845-07-3 CAPLUS
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 8-fluoro-1,2,5,6-tetrahydro-6-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

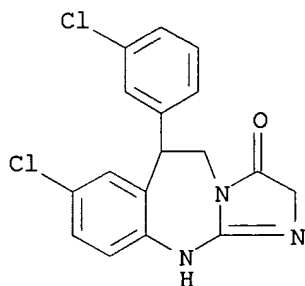


Ex. 13

● HCl

RN 97845-10-8 CAPLUS
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 8-chloro-6-(3-chlorophenyl)-

1,2,5,6-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)



Ex 14

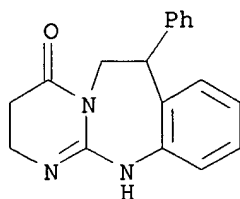
● HCl

IT 97844-36-5P 97844-37-6P 97844-38-7P
 97844-39-8P 97844-42-3P 97844-43-4P
 97844-44-5P 97844-46-7P 97844-48-9P
 97844-49-0P 97844-50-3P 97844-51-4P
 97844-52-5P 97844-53-6P 97844-54-7P
 97844-56-9P 97844-57-0P 97844-60-5P
 97844-61-6P 97844-63-8P 97844-85-4P
 97844-86-5P 97844-87-6P 97844-88-7P
 97844-89-8P 97844-90-1P 97844-91-2P
 97844-92-3P 97844-95-6P 97844-98-9P
 97844-99-0P 97845-01-7P 97845-02-8P
 97845-04-0P 97845-05-1P 97845-06-2P
 97845-09-5P 97845-12-0P 97866-88-1P
 97906-26-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 97844-36-5 CAPLUS

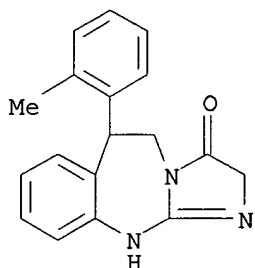
CN Pyrimido[2,1-b][1,3]benzodiazepin-4(1H)-one, 2,3,6,7-tetrahydro-7-phenyl-
 (9CI) (CA INDEX NAME)



Ex 15

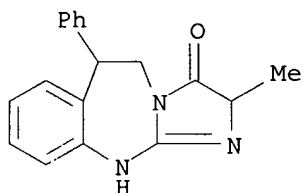
RN 97844-37-6 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-6-(2-methylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



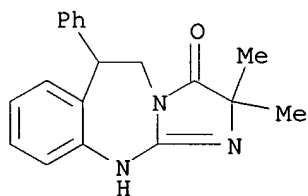
● HCl

RN 97844-38-7 CAPLUS
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-2-methyl-6-phenyl-, (2S-cis)- (9CI) (CA INDEX NAME)



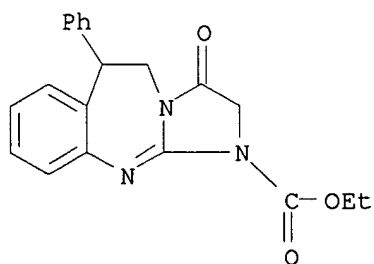
Ex. 16

RN 97844-39-8 CAPLUS
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-2,2-dimethyl-6-phenyl- (9CI) (CA INDEX NAME)



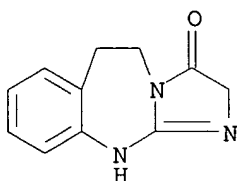
Ex 17

RN 97844-42-3 CAPLUS
CN 1H-Imidazo[2,1-b][1,3]benzodiazepine-1-carboxylic acid, 2,3,5,6-tetrahydro-3-oxo-6-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



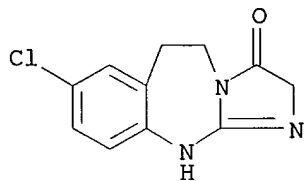
Ex. 18

RN 97844-43-4 CAPLUS
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro- (9CI) (CA INDEX NAME)



Ex 19

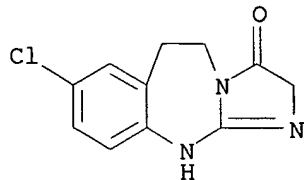
RN 97844-44-5 CAPLUS
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 8-chloro-1,2,5,6-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)



Ex. 20

● HCl

RN 97844-46-7 CAPLUS
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 8-chloro-1,2,5,6-tetrahydro- (9CI) (CA INDEX NAME)

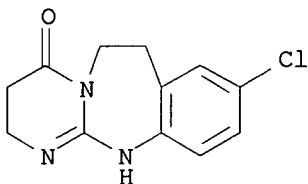


Ex. 21
22

10/019,683

RN 97844-48-9 CAPLUS

CN Pyrimido[2,1-b][1,3]benzodiazepin-4(1H)-one, 9-chloro-2,3,6,7-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)

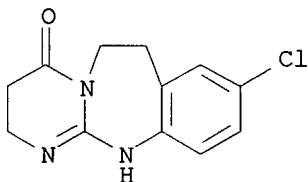


Ex. 23

● HCl

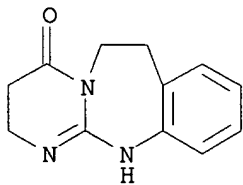
RN 97844-49-0 CAPLUS

CN Pyrimido[2,1-b][1,3]benzodiazepin-4(1H)-one, 9-chloro-2,3,6,7-tetrahydro- (9CI) (CA INDEX NAME)



RN 97844-50-3 CAPLUS

CN Pyrimido[2,1-b][1,3]benzodiazepin-4(1H)-one, 2,3,6,7-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)

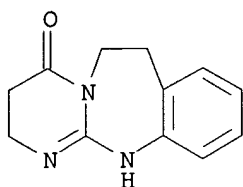


Ex. 24

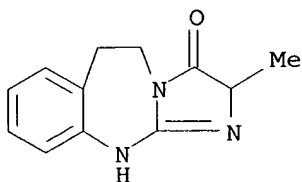
● HCl

RN 97844-51-4 CAPLUS

CN Pyrimido[2,1-b][1,3]benzodiazepin-4(1H)-one, 2,3,6,7-tetrahydro- (9CI) (CA INDEX NAME)

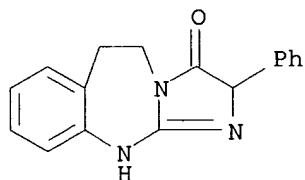


RN 97844-52-5 CAPLUS
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-2-methyl-
(9CI) (CA INDEX NAME)



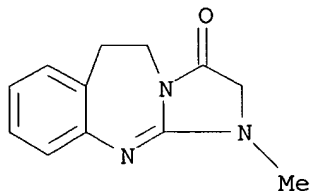
Ex. 25

RN 97844-53-6 CAPLUS
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-2-phenyl-
(9CI) (CA INDEX NAME)



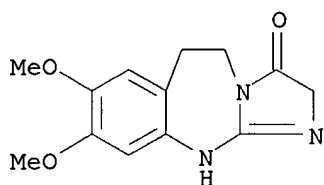
Ex. 26

RN 97844-54-7 CAPLUS
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-1-methyl-
(9CI) (CA INDEX NAME)



Ex. 27

RN 97844-56-9 CAPLUS
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-8,9-
dimethoxy-, monohydrochloride (9CI) (CA INDEX NAME)

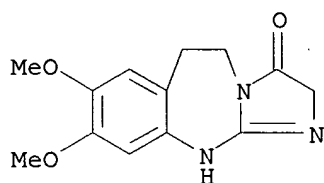


Ex. 29

● HCl

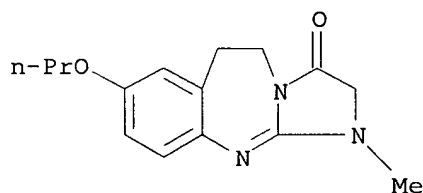
RN 97844-57-0 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-8,9-dimethoxy- (9CI) (CA INDEX NAME)



RN 97844-60-5 CAPLUS

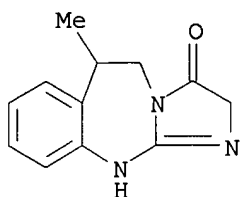
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-1-methyl-8-propoxy- (9CI) (CA INDEX NAME)



Ex. 31

RN 97844-61-6 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-6-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

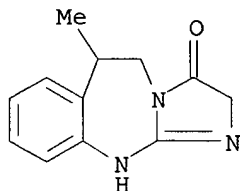


Ex. 32

● HCl

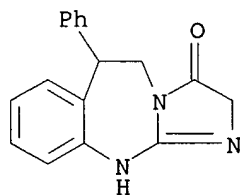
RN 97844-63-8 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-6-methyl-
(9CI) (CA INDEX NAME)



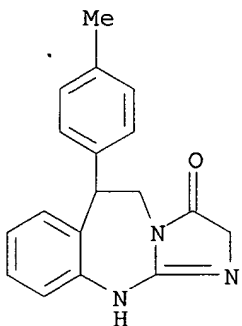
RN 97844-85-4 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-6-phenyl-
(9CI) (CA INDEX NAME)



RN 97844-86-5 CAPLUS

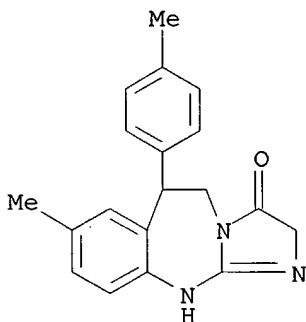
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-6-(4-methylphenyl)- (9CI) (CA INDEX NAME)



Ex 2

RN 97844-87-6 CAPLUS

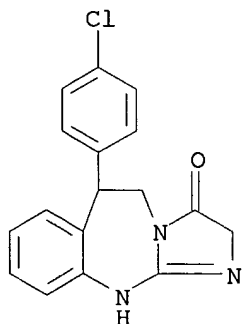
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-8-methyl-6-(4-methylphenyl)- (9CI) (CA INDEX NAME)



Ex 3

RN 97844-88-7 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 6-(4-chlorophenyl)-1,2,5,6-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)

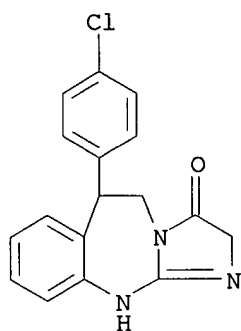


Ex 4
8

● HCl

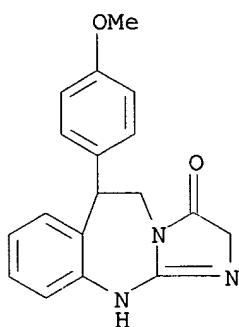
RN 97844-89-8 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 6-(4-chlorophenyl)-1,2,5,6-tetrahydro- (9CI) (CA INDEX NAME)



RN 97844-90-1 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-6-(4-methoxyphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

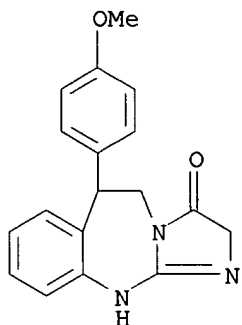


Ex 5

● HCl

RN 97844-91-2 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-6-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

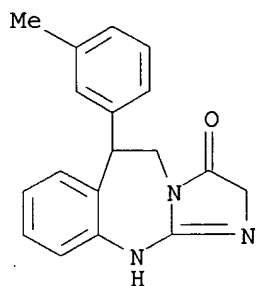


RN 97844-92-3 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-6-(3-

10/019,683

methylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

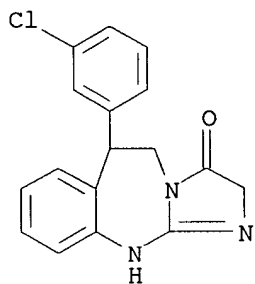


Ex. 6

● HCl

RN 97844-95-6 CAPLUS

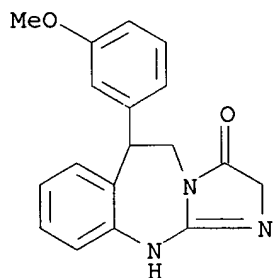
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 6-(3-chlorophenyl)-1,2,5,6-tetrahydro- (9CI) (CA INDEX NAME)



Ex 7

RN 97844-98-9 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-6-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)

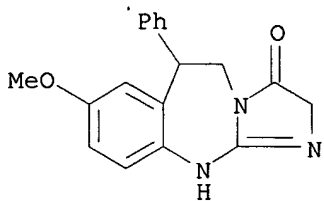


Ex. 9

RN 97844-99-0 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-8-methoxy-6-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

10/019,683

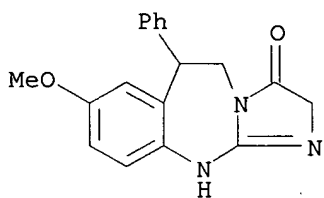


Ex. 10

● HCl

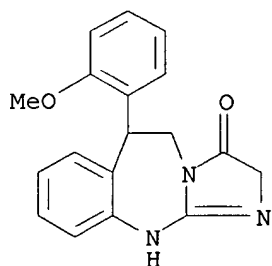
RN 97845-01-7 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-8-methoxy-6-phenyl- (9CI) (CA INDEX NAME)



RN 97845-02-8 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-6-(2-methoxyphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



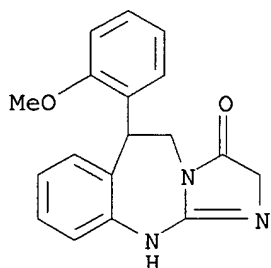
Ex. 11

● HCl

RN 97845-04-0 CAPLUS

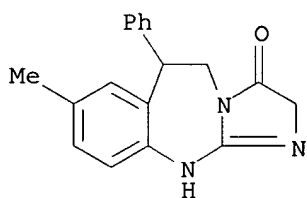
CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-6-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)

10/019,683



RN 97845-05-1 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-8-methyl-6-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

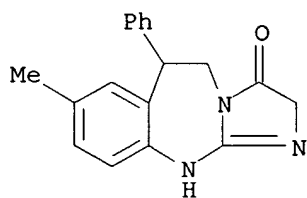


Ex 12

● HCl

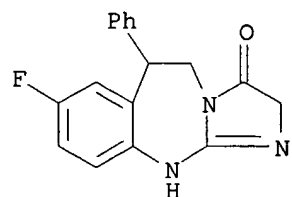
RN 97845-06-2 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-8-methyl-6-phenyl- (9CI) (CA INDEX NAME)



RN 97845-09-5 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 8-fluoro-1,2,5,6-tetrahydro-6-phenyl- (9CI) (CA INDEX NAME)

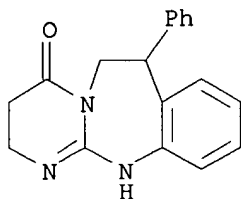


Ex. 13

10/019,683

RN 97845-12-0 CAPLUS

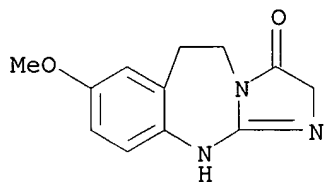
CN Pyrimido[2,1-b][1,3]benzodiazepin-4(1H)-one, 2,3,6,7-tetrahydro-7-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

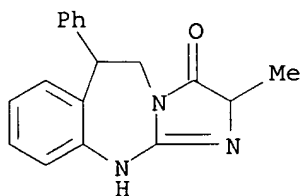
RN 97866-88-1 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-8-methoxy- (9CI) (CA INDEX NAME)



RN 97906-26-8 CAPLUS

CN 3H-Imidazo[2,1-b][1,3]benzodiazepin-3-one, 1,2,5,6-tetrahydro-2-methyl-6-phenyl-, (2S-trans)- (9CI) (CA INDEX NAME)



Ex 16

10/019,683

~~104~~ ANSWER 26 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:149293 CAPLUS

DOCUMENT NUMBER: 102:149293

TITLE: Triazolo[2,3-c][1,3]benzodiazepines and their
therapeutical use

INVENTOR(S): Vlattas, Isidoros

PATENT ASSIGNEE(S): Ciba-Geigy A.-G. , Switz.

SOURCE: Eur. Pat. Appl., 45 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

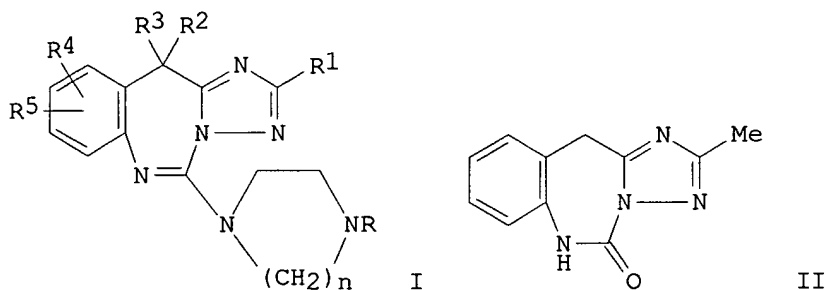
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| EP 129509 | A2 | 19841227 | EP 1984-810264 | 19840529 |
| EP 129509 | A3 | 19850911 | | |
| EP 129509 | B1 | 19890823 | | |
| R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE | | | | |
| AT 45740 | E | 19890915 | AT 1984-810264 | 19840529 |
| DK 8402764 | A | 19841207 | DK 1984-2764 | 19840604 |
| FI 8402228 | A | 19841207 | FI 1984-2228 | 19840604 |
| FI 78098 | B | 19890228 | | |
| FI 78098 | C | 19890612 | | |
| CA 1215044 | A1 | 19861209 | CA 1984-455776 | 19840604 |
| IL 72015 | A1 | 19871231 | IL 1984-72015 | 19840604 |
| NO 8402254 | A | 19841207 | NO 1984-2254 | 19840605 |
| NO 162070 | B | 19890724 | | |
| NO 162070 | C | 19891101 | | |
| AU 8429106 | A1 | 19841213 | AU 1984-29106 | 19840605 |
| AU 574075 | B2 | 19880630 | | |
| ZA 8404186 | A | 19850227 | ZA 1984-4186 | 19840605 |
| DD 220310 | A5 | 19850327 | DD 1984-263805 | 19840605 |
| HU 34488 | A2 | 19850328 | HU 1984-2181 | 19840605 |
| HU 190930 | B | 19861228 | | |
| ES 533135 | A1 | 19850801 | ES 1984-533135 | 19840605 |
| JP 60006689 | A2 | 19850114 | JP 1984-114697 | 19840606 |
| JP 03054669 | B4 | 19910820 | | |
| US 4595535 | A | 19860617 | US 1984-643136 | 19840822 |
| PRIORITY APPLN. INFO.: | | | US 1983-501328 | A 19830606 |
| | | | EP 1984-810264 | A 19840529 |

OTHER SOURCE(S): MARPAT 102:149293

GI



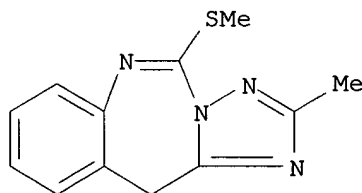
AB The title compds. [I; R = H, alkenyl, alkynyl, alkanoyl, (un)substituted alkyl, alkoxy, carbonyl; R1 = H, alkoxy, alkylthio, alkoxy, acyloxy, OH, halo, cyano, F3C, CO2H, carbamoyl, (un)substituted alkyl; R2, R3 = H, alkyl; R4, R5 = H, alkyl, alkoxy, alkylthio, OH, halo, F3C, sulfamoyl; n = 2, 3] were prepared. Thus, 2-O2NC6H4CH2CN was treated with EtOH and HCl to give 2-O2NC6H4CH2C(NH)OEt which was cyclocondensed with AcNHNH2 to give 3-methyl-5-(o-nitrobenzyl)-1,2,4-triazole. This was reduced and cyclocondensed with 1,1'-carbonyldiimidazole to give triazolobenzodiazepinone II, which was converted in 2 steps to I (R = R1 = Me, R2-R5 = H) (III). III had antipsychotic activity in rats at ≤ 1.0 mg/kg orally and inhibited histamine activation by adenylate cyclase with an IC50 of $\text{apprx. } 3 \times 10^{-6}$ M.

IT 95614-51-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with methylpiperazine)

RN 95614-51-0 CAPLUS

CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 2-methyl-5-(methylthio)-
(9CI) (CA INDEX NAME)

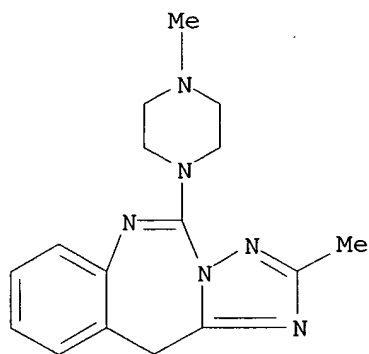


IT 95634-82-5P 95634-83-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antihistaminic and tranquilizer activity of)

RN 95634-82-5 CAPLUS

CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 2-methyl-5-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

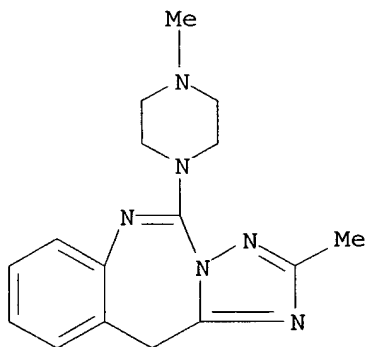


RN 95634-83-6 CAPLUS
 CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 2-methyl-5-(4-methyl-1-piperazinyl)-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 95634-82-5

CMF C16 H20 N6

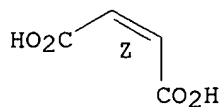


CM 2

CRN 110-16-7

CMF C4 H4 O4

Double bond geometry as shown.



IT 95614-49-6P

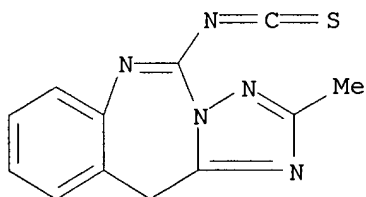
RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and condensation of, with methylpiperazine)

RN 95614-49-6 CAPLUS

CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 5-isothiocyanato-2-methyl-

10/019,683

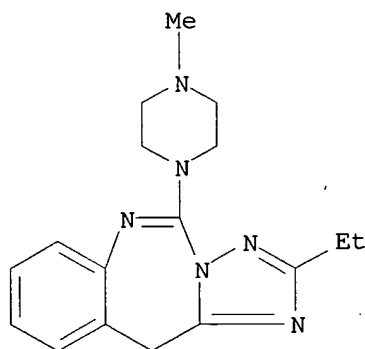
(9CI) (CA INDEX NAME)



IT 95634-85-8P 95634-87-0P 95634-89-2P
95634-91-6P 95634-93-8P 95663-86-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 95634-85-8 CAPLUS
CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 2-ethyl-5-(4-methyl-1-piperazinyl)-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

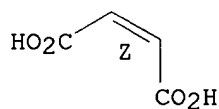
CRN 95634-84-7
CMF C17 H22 N6



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



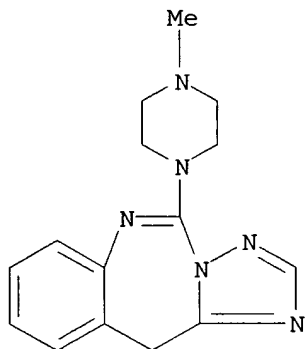
RN 95634-87-0 CAPLUS
CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 5-(4-methyl-1-piperazinyl)-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

10/019,683

CM 1

CRN 95634-86-9

CMF C15 H18 N6

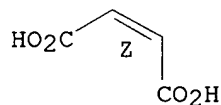


CM 2

CRN 110-16-7

CMF C4 H4 O4

Double bond geometry as shown.



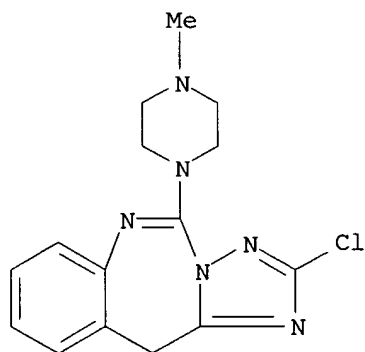
RN 95634-89-2 CAPLUS

CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 2-chloro-5-(4-methyl-1-piperazinyl)-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 95634-88-1

CMF C15 H17 Cl N6



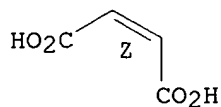
10/019,683

CM 2

CRN 110-16-7

CMF C4 H4 O4

Double bond geometry as shown.



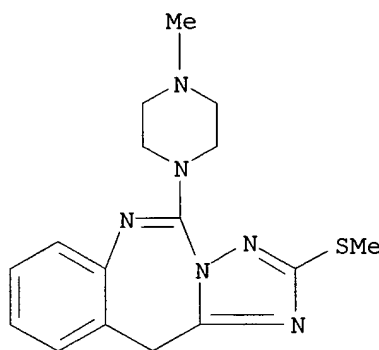
RN 95634-91-6 CAPLUS

CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 5-(4-methyl-1-piperazinyl)-2-(methylthio)-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 95634-90-5

CMF C16 H20 N6 S

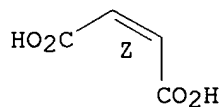


CM 2

CRN 110-16-7

CMF C4 H4 O4

Double bond geometry as shown.



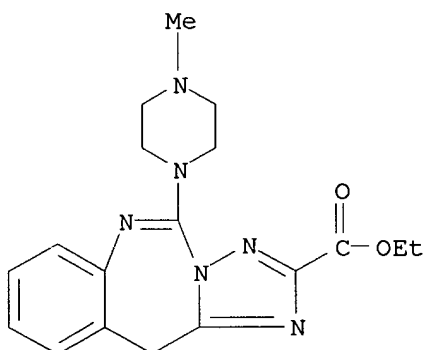
RN 95634-93-8 CAPLUS

CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine-2-carboxylic acid, 5-(4-methyl-1-piperazinyl)-, ethyl ester, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

10/019,683

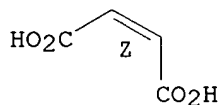
CRN 95634-92-7
CMF C18 H22 N6 O2



CM 2

CRN 110-16-7
CMF C4 H4 O4

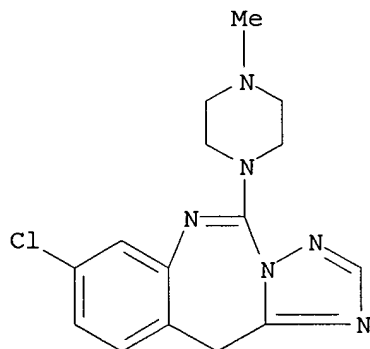
Double bond geometry as shown.



RN 95663-86-8 CAPLUS
CN 11H-[1,2,4]Triazolo[1,5-c][1,3]benzodiazepine, 8-chloro-5-(4-methyl-1-piperazinyl)-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 95663-85-7
CMF C15 H17 Cl N6



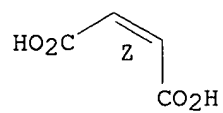
10/019,683

CM 2

CRN 110-16-7

CMF C4 H4 O4

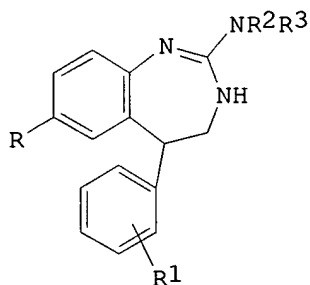
Double bond geometry as shown.



L14 ANSWER 27 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:62284 CAPLUS
 DOCUMENT NUMBER: 102:62284
 TITLE: 2-Amino-5-phenyl-1,3-benzodiazepines and medicines containing
 INVENTOR(S): Bayssat, Michel; Ferrand, Gerard; Depin, Jean-claude
 PATENT ASSIGNEE(S): LIPHA, Lyonnaise Industrielle Pharmaceutique, Fr.
 SOURCE: Fr. Demande, 22 pp.
 CODEN: FRXXBL
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------------------|----------|-----------------|------------|
| FR 2540871 | A1 | 19840817 | FR 1983-2475 | 19830216 |
| FR 2540871 | B1 | 19860110 | | |
| ZA 8400765 | A | 19840926 | ZA 1984-765 | 19840201 |
| EP 117794 | A1 | 19840905 | EP 1984-400233 | 19840203 |
| R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE | | | | |
| CA 1213585 | A1 | 19861104 | CA 1984-446858 | 19840206 |
| US 4554273 | A | 19851119 | US 1984-578046 | 19840207 |
| ES 529728 | A1 | 19841101 | ES 1984-529728 | 19840215 |
| JP 59155373 | A2 | 19840904 | JP 1984-26197 | 19840216 |
| PRIORITY APPLN. INFO.: | | | FR 1983-2475 | A 19830216 |
| OTHER SOURCE(S): | MARPAT 102:62284 | | | |
| GI | | | | |



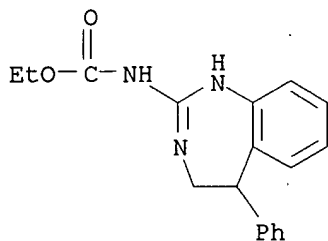
I

AB Title compds. I [R and R1 are H, halo, alkyl, alkoxy; R2 = H, alkyl; R3 = H, alkyl, cycloalkyl, arylalkyl, heteroarylalkyl, (dialkylamino)alkyl, dialkylamino, carbalkoxy, cyano; or NR2R3 form a heterocycle], which were prepared, exhibited antidepressant activity. 2-Methylthio-5-phenyl-4,5-dihydro-3H-1,3-benzodiazepine hydriodide was heated with NH3 in EtOH, and the mixture was made alkaline to give I (R = R1 = R2 = R3 = H).

IT 94568-63-5P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation and antidepressant activity of)

RN 94568-63-5 CAPLUS

CN Carbamic acid, (4,5-dihydro-5-phenyl-1H-1,3-benzodiazepin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

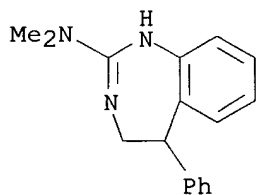


IT 94568-16-8P 94568-17-9P 94568-18-0P
 94568-19-1P 94568-20-4P 94568-21-5P
 94568-22-6P 94568-23-7P 94568-24-8P
 94568-25-9P 94568-26-0P 94568-27-1P
 94568-28-2P 94568-30-6P 94568-31-7P
 94568-32-8P 94568-33-9P 94568-34-0P
 94568-35-1P 94568-36-2P 94568-37-3P
 94568-38-4P 94568-39-5P 94568-40-8P
 94568-41-9P 94568-42-0P 94568-43-1P
 94568-44-2P 94568-45-3P 94568-46-4P
 94568-48-6P 94568-50-0P 94568-52-2P
 94568-53-3P 94568-54-4P 94568-56-6P
 94568-57-7P 94568-58-8P 94568-59-9P
 94568-60-2P 94568-61-3P 94568-62-4P
 94568-64-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 94568-16-8 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N,N-dimethyl-5-phenyl- (9CI)
 (CA INDEX NAME)



RN 94568-17-9 CAPLUS

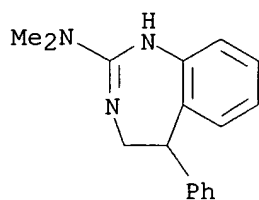
CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N,N-dimethyl-5-phenyl-,
 ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 94568-16-8

CMF C17 H19 N3

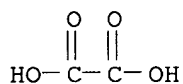
10/019,683



CM 2

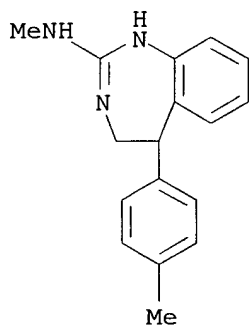
CRN 144-62-7

CMF C2 H2 O4



RN 94568-18-0 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-methyl-5-(4-methylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

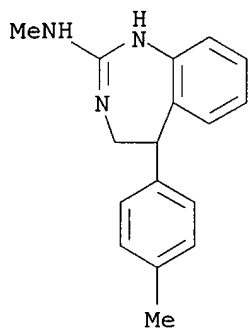


● HCl

RN 94568-19-1 CAPLUS

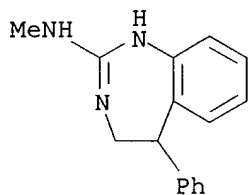
CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-methyl-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)

10/019,683



RN 94568-20-4 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-methyl-5-phenyl- (9CI) (CA INDEX NAME)



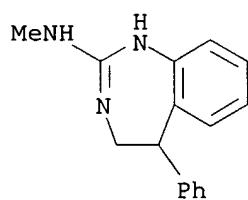
RN 94568-21-5 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-methyl-5-phenyl-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 94568-20-4

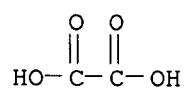
CMF C16 H17 N3



CM 2

CRN 144-62-7

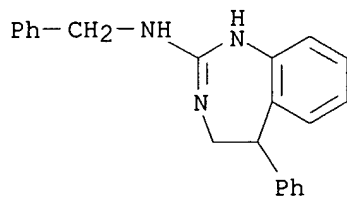
CMF C2 H2 O4



10/019,683

RN 94568-22-6 CAPLUS

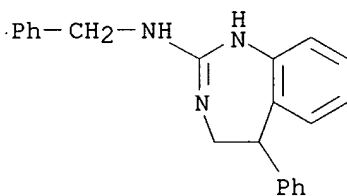
CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-5-phenyl-N-(phenylmethyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 94568-23-7 CAPLUS

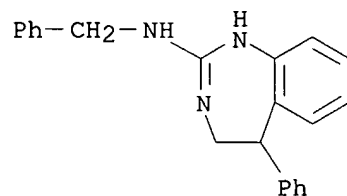
CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-5-phenyl-N-(phenylmethyl)-,
monohydriodide (9CI) (CA INDEX NAME)



● HI

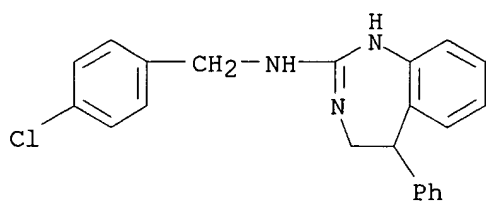
RN 94568-24-8 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-5-phenyl-N-(phenylmethyl)- (9CI)
(CA INDEX NAME)



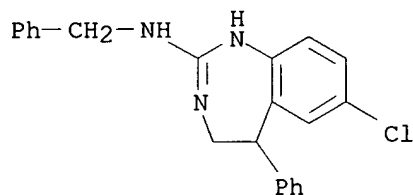
RN 94568-25-9 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, N-[(4-chlorophenyl)methyl]-4,5-dihydro-5-
phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



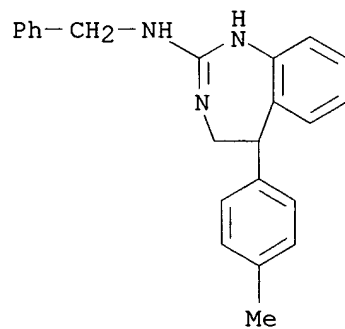
● HCl

RN 94568-26-0 CAPLUS
 CN 1H-1,3-Benzodiazepin-2-amine, 7-chloro-4,5-dihydro-5-phenyl-N-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

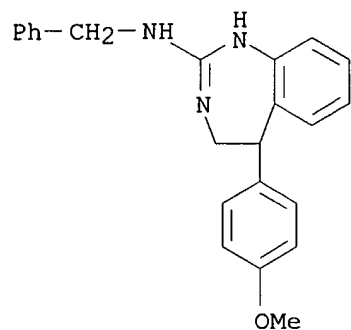
RN 94568-27-1 CAPLUS
 CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-5-(4-methylphenyl)-N-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

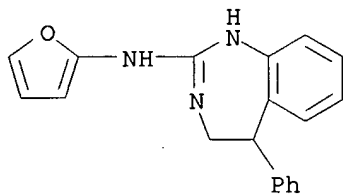
RN 94568-28-2 CAPLUS
 CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-5-(4-methoxyphenyl)-N-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

10/019,683

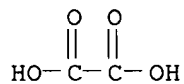


● HCl

RN 94568-30-6 CAPLUS
CN 1H-1,3-Benzodiazepin-2-amine, N-2-furanyl-4,5-dihydro-5-phenyl-,
ethanedioate (2:1) (9CI) (CA INDEX NAME)
CM 1
CRN 94568-29-3
CMF C19 H17 N3 O

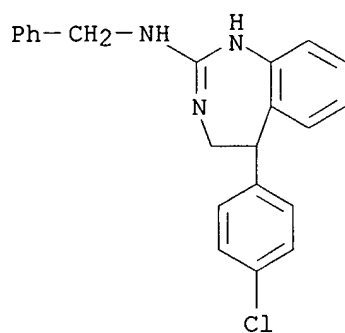


CM 2
CRN 144-62-7
CMF C2 H2 O4



RN 94568-31-7 CAPLUS
CN 1H-1,3-Benzodiazepin-2-amine, 5-(4-chlorophenyl)-4,5-dihydro-N-(
phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

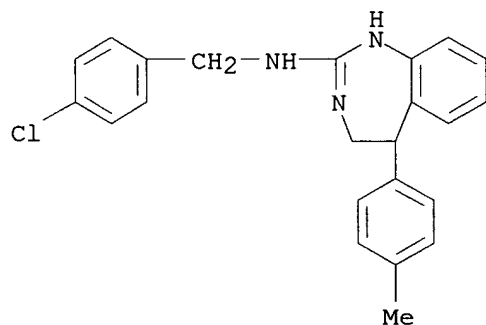
10/019,683



● HCl

RN 94568-32-8 CAPLUS

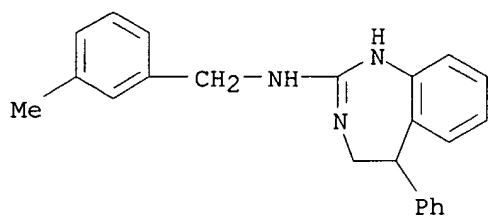
CN 1H-1,3-Benzodiazepin-2-amine, N-[(4-chlorophenyl)methyl]-4,5-dihydro-5-(4-methylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

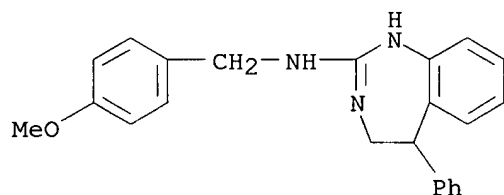
RN 94568-33-9 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-[(3-methylphenyl)methyl]-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



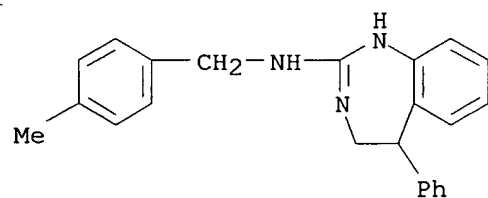
● HCl

RN 94568-34-0 CAPLUS
 CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-[(4-methoxyphenyl)methyl]-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



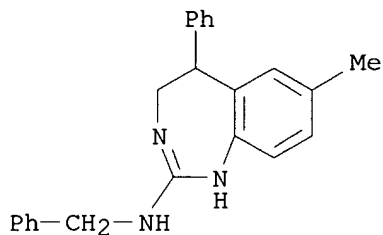
● HCl

RN 94568-35-1 CAPLUS
 CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-[(4-methylphenyl)methyl]-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



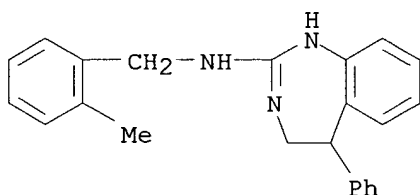
● HCl

RN 94568-36-2 CAPLUS
 CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-7-methyl-5-phenyl-N-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



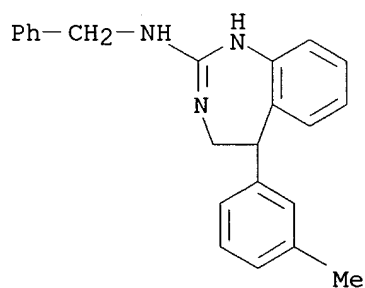
● HCl

RN 94568-37-3 CAPLUS
 CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-[(2-methylphenyl)methyl]-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



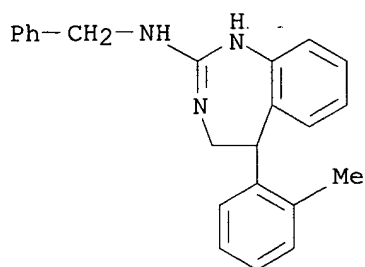
● HCl

RN 94568-38-4 CAPLUS
 CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-5-(3-methylphenyl)-N-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



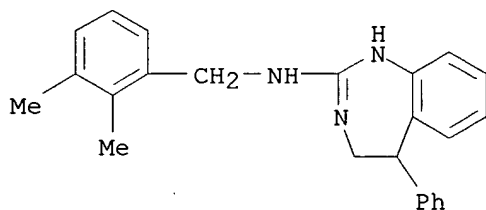
● HCl

RN 94568-39-5 CAPLUS
 CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-5-(2-methylphenyl)-N-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



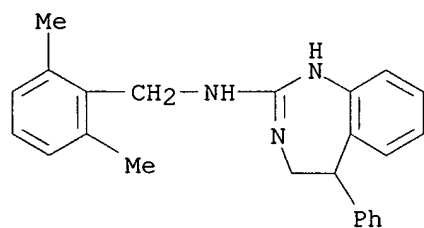
● HCl

RN 94568-40-8 CAPLUS
 CN 1H-1,3-Benzodiazepin-2-amine, N-[(2,3-dimethylphenyl)methyl]-4,5-dihydro-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

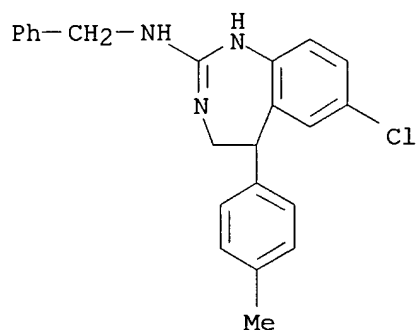
RN 94568-41-9 CAPLUS
 CN 1H-1,3-Benzodiazepin-2-amine, N-[(2,6-dimethylphenyl)methyl]-4,5-dihydro-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 94568-42-0 CAPLUS
 CN 1H-1,3-Benzodiazepin-2-amine, 7-chloro-4,5-dihydro-5-(4-methylphenyl)-N-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

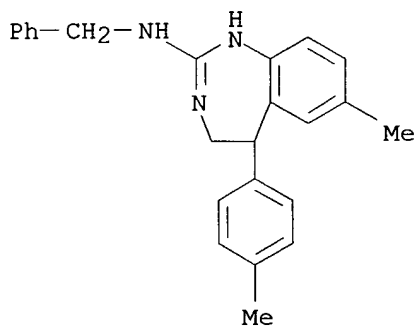
10/019,683



● HCl

RN 94568-43-1 CAPLUS

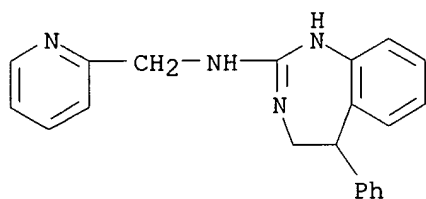
CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-7-methyl-5-(4-methylphenyl)-N-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

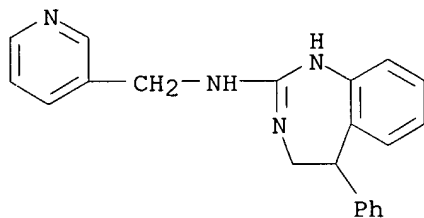
RN 94568-44-2 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-5-phenyl-N-(2-pyridinylmethyl)-, dihydrochloride (9CI) (CA INDEX NAME)



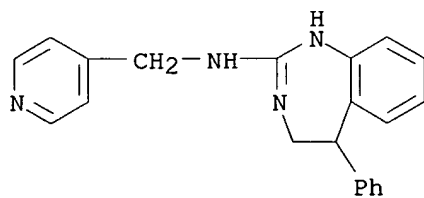
●2 HCl

RN 94568-45-3 CAPLUS
CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-5-phenyl-N-(3-pyridinylmethyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 94568-46-4 CAPLUS
CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-5-phenyl-N-(4-pyridinylmethyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

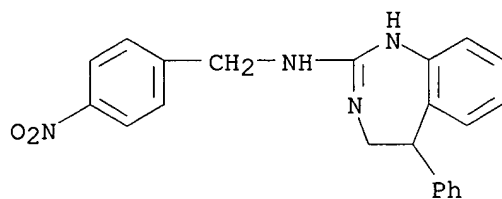
RN 94568-48-6 CAPLUS
CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-[(4-nitrophenyl)methyl]-5-phenyl-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 94568-47-5

10/019,683

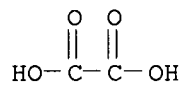
CMF C22 H20 N4 O2



CM 2

CRN 144-62-7

CMF C2 H2 O4



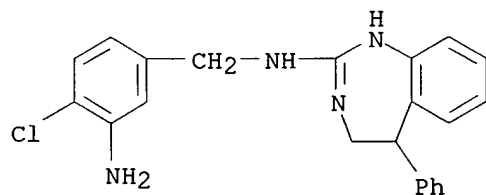
RN 94568-50-0 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, N-[(3-amino-4-chlorophenyl)methyl]-4,5-dihydro-5-phenyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 94568-49-7

CMF C22 H21 Cl N4

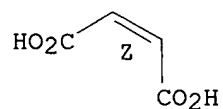


CM 2

CRN 110-16-7

CMF C4 H4 O4

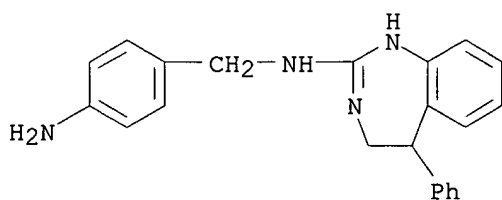
Double bond geometry as shown.



RN 94568-52-2 CAPLUS

10/019,683

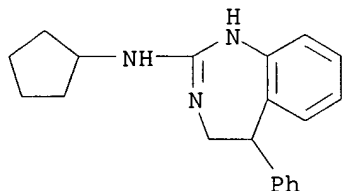
CN 1H-1,3-Benzodiazepin-2-amine, N-[(4-aminophenyl)methyl]-4,5-dihydro-5-phenyl-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

RN 94568-53-3 CAPLUS

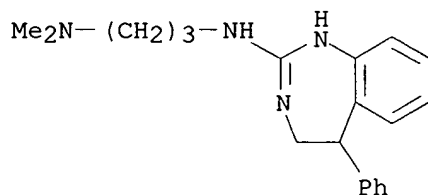
CN 1H-1,3-Benzodiazepin-2-amine, N-cyclopentyl-4,5-dihydro-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 94568-54-4 CAPLUS

CN 1,3-Propanediamine, N'-(4,5-dihydro-5-phenyl-1H-1,3-benzodiazepin-2-yl)-N,N-dimethyl-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

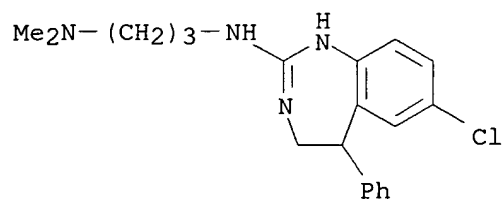
RN 94568-56-6 CAPLUS

CN 1,3-Propanediamine, N'-(7-chloro-4,5-dihydro-5-phenyl-1H-1,3-benzodiazepin-2-yl)-N,N-dimethyl-, ethanedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

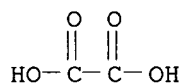
10/019,683

CRN 94568-55-5
CMF C20 H25 Cl N4

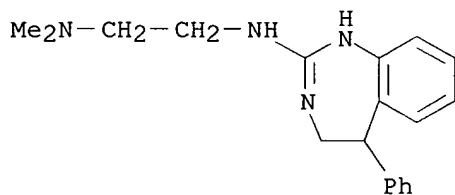


CM 2

CRN 144-62-7
CMF C2 H2 O4



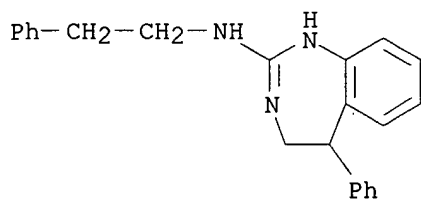
RN 94568-57-7 CAPLUS
CN 1,2-Ethanediamine, N'-(4,5-dihydro-5-phenyl-1H-1,3-benzodiazepin-2-yl)-N,N-dimethyl-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 94568-58-8 CAPLUS
CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-5-phenyl-N-(2-phenylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

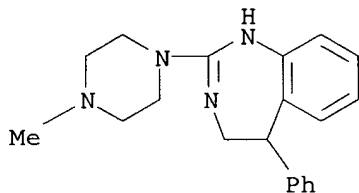
10/019,683



● HCl

RN 94568-59-9 CAPLUS

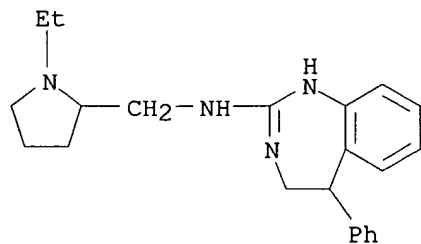
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(4-methyl-1-piperazinyl)-5-phenyl-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 94568-60-2 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, N-[(1-ethyl-2-pyrrolidinyl)methyl]-4,5-dihydro-5-phenyl-, dihydrochloride (9CI) (CA INDEX NAME)



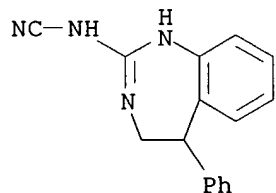
●2 HCl

RN 94568-61-3 CAPLUS

CN Benzenemethanol, α -[[[4,5-dihydro-5-phenyl-1H-1,3-benzodiazepin-2-yl)amino]methyl]- (9CI) (CA INDEX NAME)

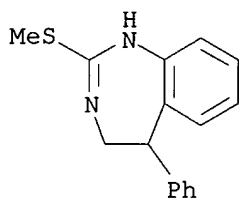
O[C@@H](c1ccccc1)CNc2nc3c(c[nH]3c4ccccc42)Cc5ccccc5CN(C)N=C1NC(=N1Cc2ccccc2)Cc3ccccc3

| | | | |
|----|--|--------|--|
| RN | 94568-64-6 | CAPLUS | |
| CN | Cyanamide, (4,5-dihydro-5-phenyl-1H-1,3-benzodiazepin-2-yl)- (9CI) (CA INDEX NAME) | | |



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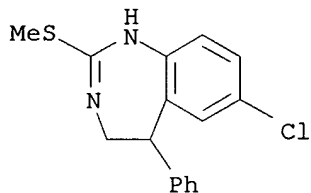
10/019,683



● HI

RN 90156-41-5 CAPLUS

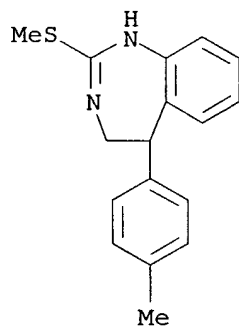
CN 1H-1,3-Benzodiazepine, 7-chloro-4,5-dihydro-2-(methylthio)-5-phenyl-,
monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 90156-43-7 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-(4-methylphenyl)-2-(methylthio)-,
monohydriodide (9CI) (CA INDEX NAME)



● HI

IT 90156-45-9 94568-07-7 94568-09-9
94568-11-3 94568-13-5 94594-64-6
94594-65-7

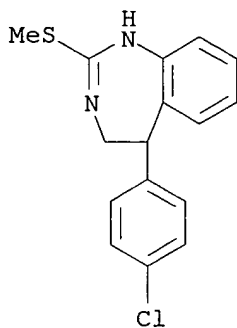
10/019,683

RL: PROC (Process)

(substitution of, with ammonia and benzylamine)

RN 90156-45-9 CAPLUS

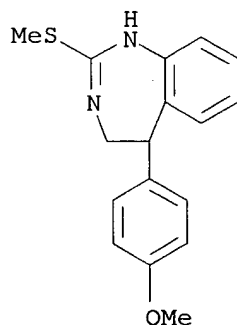
CN 1H-1,3-Benzodiazepine, 5-(4-chlorophenyl)-4,5-dihydro-2-(methylthio)-,
monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 94568-07-7 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-(4-methoxyphenyl)-2-(methylthio)-,
monohydriodide (9CI) (CA INDEX NAME)

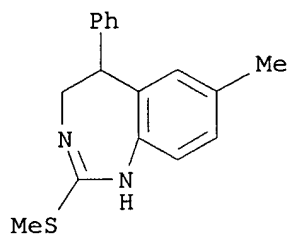


● HI

RN 94568-09-9 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-7-methyl-2-(methylthio)-5-phenyl-,
monohydriodide (9CI) (CA INDEX NAME)

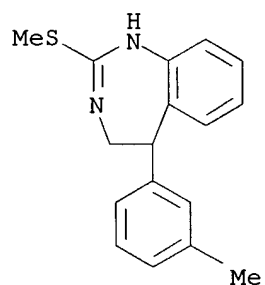
10/019,683



● HI

RN 94568-11-3 CAPLUS

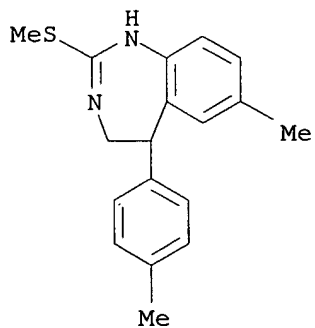
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-(3-methylphenyl)-2-(methylthio)-, monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 94568-13-5 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-7-methyl-5-(4-methylphenyl)-2-(methylthio)-, monohydriodide (9CI) (CA INDEX NAME)

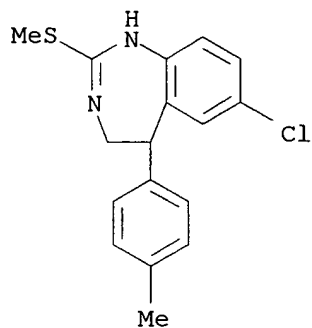


● HI

10/019,683

RN 94594-64-6 CAPLUS

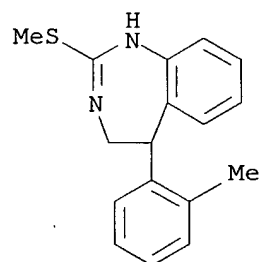
CN 1H-1,3-Benzodiazepine, 7-chloro-4,5-dihydro-5-(4-methylphenyl)-2-(methylthio)-, monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 94594-65-7 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-(2-methylphenyl)-2-(methylthio)-, monohydriodide (9CI) (CA INDEX NAME)



● HI

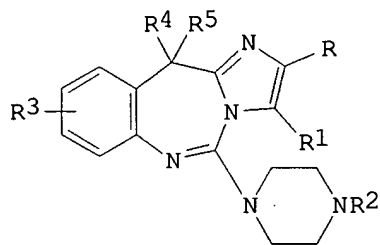
10/019,683

114 ANSWER 28 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

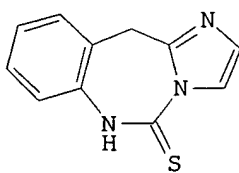
ACCESSION NUMBER: 1984:611186 CAPLUS
DOCUMENT NUMBER: 101:211186
TITLE: 5-Diazacycloalkylimidazo[1,2-c][1,3]benzodiazepines
INVENTOR(S): Vlattas, Isidoros
PATENT ASSIGNEE(S): Ciba-Geigy Corp. , USA
SOURCE: U.S., 12 pp. Cont.-in-part of U.S. Ser. No. 328,274,
abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| US 4460587 | A | 19840717 | US 1982-444957 | 19821129 |
| US 4459232 | A | 19840710 | US 1982-417746 | 19820913 |
| US 4460508 | A | 19840717 | US 1982-417747 | 19820913 |
| FI 8204170 | A | 19830608 | FI 1982-4170 | 19821103 |
| GB 2115407 | A1 | 19830907 | GB 1982-34334 | 19821202 |
| GB 2115407 | B2 | 19850724 | | |
| ES 517912 | A1 | 19841201 | ES 1982-517912 | 19821203 |
| CA 1180011 | A1 | 19841225 | CA 1982-416953 | 19821203 |
| DK 8205402 | A | 19830608 | DK 1982-5402 | 19821206 |
| NO 8204090 | A | 19830608 | NO 1982-4090 | 19821206 |
| AU 8291315 | A1 | 19830616 | AU 1982-91315 | 19821206 |
| JP 58109489 | A2 | 19830629 | JP 1982-212828 | 19821206 |
| ZA 8208954 | A | 19830928 | ZA 1982-8954 | 19821206 |
| DD 203547 | A5 | 19831026 | DD 1982-245615 | 19821206 |
| HU 27368 | O | 19831028 | HU 1982-3911 | 19821206 |
| HU 187191 | B | 19851128 | | |
| ES 530125 | A1 | 19851101 | ES 1984-530125 | 19840228 |
| US 4507311 | A | 19850326 | US 1984-602649 | 19840423 |
| PRIORITY APPLN. INFO.: | | | US 1981-328274 | A2 19811207 |
| | | | US 1982-444957 | A3 19821129 |

OTHER SOURCE(S): CASREACT 101:211186
GI



I



II

AB Piperazinylimidazobenzodiazepines I (R, R1 = H, alkyl, cyano, CO2H, alkoxy, carbonyl, carbamoyl; R2 = H, alkyl, alkoxy, hydroxyalkyl; R3 = H, alkyl, alkoxy, alkylthio, halo, CF3; R4, R5 = H, alkyl) and their N-oxides were prepared. Thus, 2-O2NC6H4Me was treated with (CO2Et)2,

followed by $\text{H}_2\text{NOH}\cdot\text{HCl}$ and acidic hydrolysis to give $2\text{-O}_2\text{NC}_6\text{H}_4\text{CH}_2\text{C}(\text{:NOH})\text{CO}_2\text{H}$, which was heated to give $2\text{-O}_2\text{NC}_6\text{H}_4\text{CH}_2\text{CN}$.
 Ethanolysis of the latter compound gave $2\text{-O}_2\text{NC}_6\text{H}_4\text{CH}_2\text{C}(\text{:NH})\text{OEt}$ which was
 cyclocondensed with $\text{H}_2\text{NCH}_2\text{CH}(\text{OMe})_2$ to give $2\text{-(2-nitrobenzyl)imidazole}$.
 This was reduced to the amino derivative and cyclocondensed with CSCl_2 to give
 imidazobenzodiazepinethione II. II was S-methylated with MeI and aminated
 with 1-methylpiperazine to give I ($\text{R} = \text{R}_1 = \text{R}_3 = \text{R}_4 = \text{R}_5 = \text{H}$, $\text{R}_2 = \text{Me}$,
 III). III at $1 + 10^{-6}\text{M}$ inhibited histamine activation of adenylate
 cyclase in guinea pig cerebral cortex vesicles by 50% and at 50 mg/kg
 orally to monkeys and rats blocked conditioned avoidance behavior.

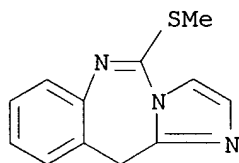
IT 87081-83-2P 87081-98-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation and amination of, by methylpiperazine)

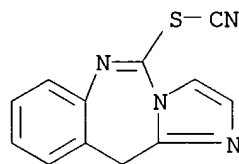
RN 87081-83-2 CAPLUS

CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(methylthio)- (9CI) (CA INDEX
 NAME)



RN 87081-98-9 CAPLUS

CN Thiocyanic acid, 11H-imidazo[1,2-c][1,3]benzodiazepin-5-yl ester (9CI)
 (CA INDEX NAME)



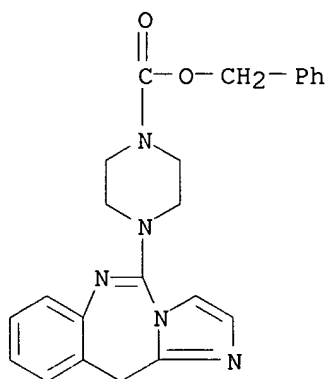
IT 92989-77-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation and deprotection of)

RN 92989-77-0 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-(11H-imidazo[1,2-c][1,3]benzodiazepin-5-yl)-
 , phenylmethyl ester (9CI) (CA INDEX NAME)

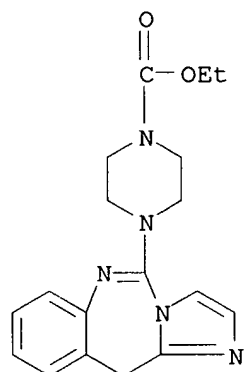


IT 87082-00-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and hydride reduction of)

RN 87082-00-6 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-(11H-imidazo[1,2-c][1,3]benzodiazepin-5-yl)-
, ethyl ester (9CI) (CA INDEX NAME)

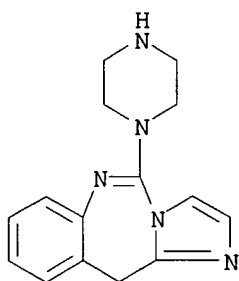


IT 87082-09-5P

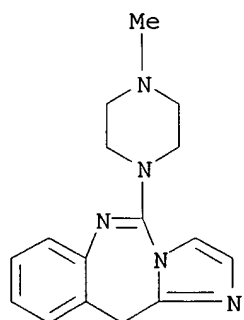
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and methylation of)

RN 87082-09-5 CAPLUS

CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(1-piperazinyl)- (9CI) (CA INDEX
NAME)

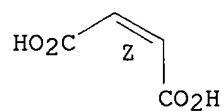


IT 87081-85-4P 87081-94-5P 87081-95-6P
 87082-03-9P 87082-04-0P 87082-05-1P
 87082-06-2P 87082-07-3P 87082-11-9P
 87082-17-5P 87092-49-7P 92976-11-9P
 92976-12-0P 92989-78-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 87081-85-4 CAPLUS
 CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(4-methyl-1-piperazinyl)-,
 (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)
 CM 1
 CRN 87081-84-3
 CMF C16 H19 N5



CM 2
 CRN 110-16-7
 CMF C4 H4 O4

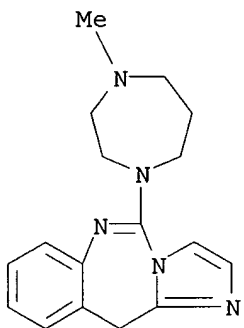
Double bond geometry as shown.



RN 87081-94-5 CAPLUS

10/019,683

CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)- (9CI) (CA INDEX NAME)



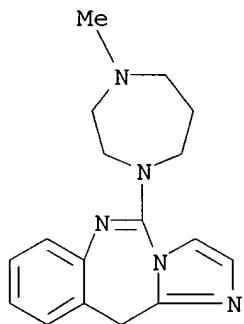
RN 87081-95-6 CAPLUS

CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 87081-94-5

CMF C17 H21 N5

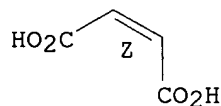


CM 2

CRN 110-16-7

CMF C4 H4 O4

Double bond geometry as shown.

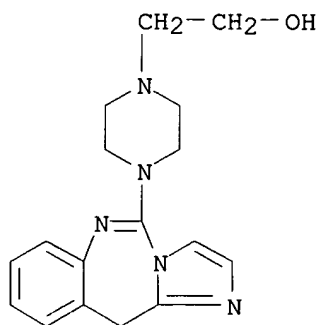


RN 87082-03-9 CAPLUS

CN 1-Piperazineethanol, 4-(11H-imidazo[1,2-c][1,3]benzodiazepin-5-yl)- (9CI)

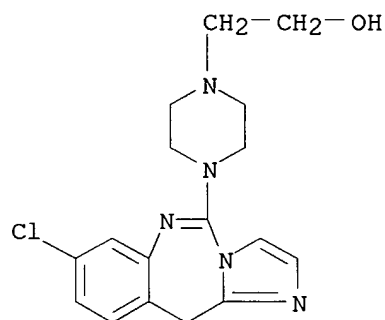
10/019,683

(CA INDEX NAME)



RN 87082-04-0 CAPLUS

CN 1-Piperazineethanol, 4-(8-chloro-11H-imidazo[1,2-c][1,3]benzodiazepin-5-yl)-, monohydrochloride (9CI) (CA INDEX NAME)

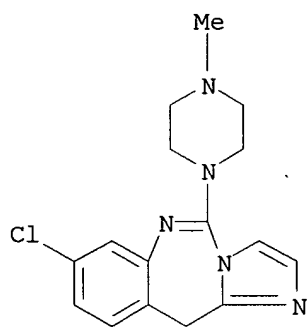


● HCl

RN 87082-05-1 CAPLUS

CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 8-chloro-5-(4-methyl-1-piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)

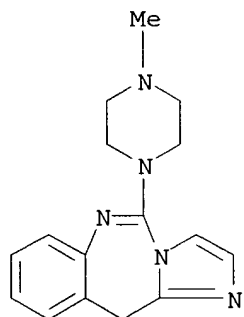
10/019,683



●2 HCl

RN 87082-06-2 CAPLUS

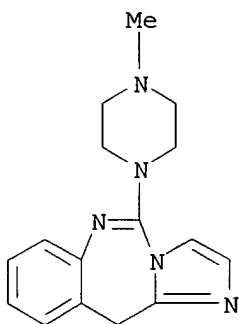
CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(4-methyl-1-piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 87082-07-3 CAPLUS

CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(4-methyl-1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

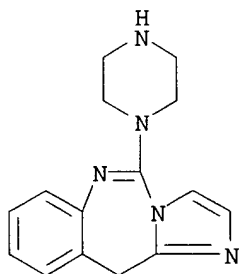


● HCl

RN 87082-11-9 CAPLUS
CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(1-piperazinyl)-,
(2Z)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

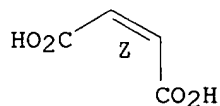
CRN 87082-09-5
CMF C15 H17 N5



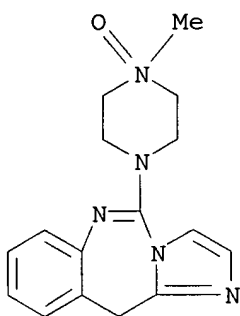
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



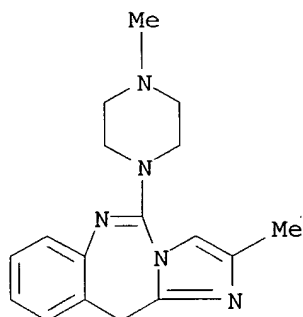
RN 87082-17-5 CAPLUS
CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(4-methyl-4-oxido-1-piperazinyl)-
(9CI) (CA INDEX NAME)



RN 87092-49-7 CAPLUS
 CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 2-methyl-5-(4-methyl-1-piperazinyl)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

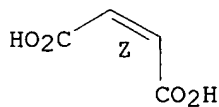
CRN 87082-14-2
 CMF C17 H21 N5



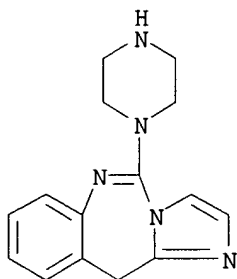
CM 2

CRN 110-16-7
 CMF C4 H4 O4

Double bond geometry as shown.

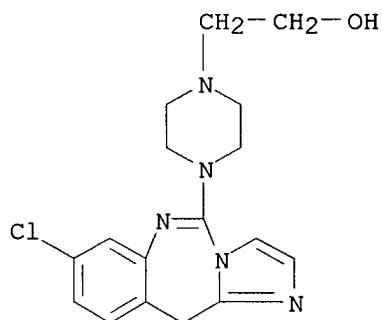


RN 92976-11-9 CAPLUS
 CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(1-piperazinyl)-, monohydrobromide (9CI) (CA INDEX NAME)

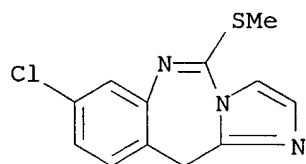


● HBr

RN 92976-12-0 CAPLUS
CN 1-Piperazineethanol, 4-(8-chloro-11H-imidazo[1,2-c][1,3]benzodiazepin-5-yl)- (9CI) (CA INDEX NAME)

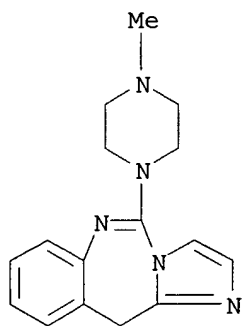


RN 92989-78-1 CAPLUS
CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 8-chloro-5-(methylthio)- (9CI) (CA INDEX NAME)



IT 87081-84-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, oxidation, and antihistaminic and neuroleptic activities of)
RN 87081-84-3 CAPLUS
CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

10/019,683



L14 ANSWER 29 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:490991 CAPLUS

DOCUMENT NUMBER: 101:90991

TITLE: 2-Anilino-5-phenyl-1,3-benzodiazepines and medicines containing them

INVENTOR(S): Bayssat, Michel; Ferrand, Gerard; Chabert, Janine

PATENT ASSIGNEE(S): LIPHA, Lyonnaise Industrielle Pharmaceutique, Fr.

SOURCE: Fr. Demande, 17 pp.

CODEN: FRXXBL

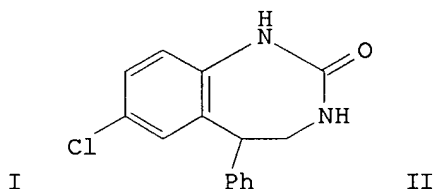
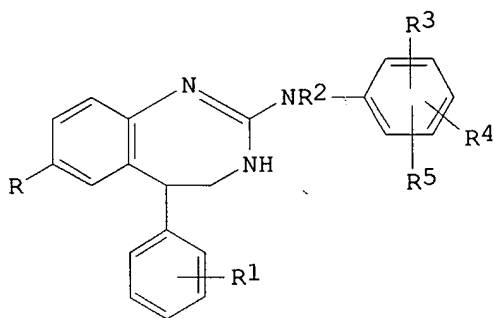
DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|--------------------------------------|-----------------|----------|
| FR 2531428 | A1 | 19840210 | FR 1982-13605 | 19820804 |
| FR 2531428 | B1 | 19850222 | | |
| PRIORITY APPLN. INFO.: | | | FR 1982-13605 | 19820804 |
| OTHER SOURCE(S): | | CASREACT 101:90991; MARPAT 101:90991 | | |
| GI | | | | |



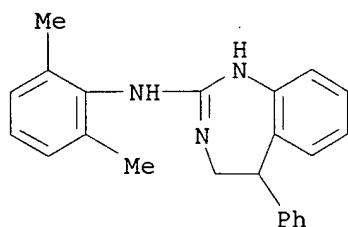
AB Title compds. I (R and R1 are H, halo, alkyl, alkoxy; R2 = H, alkyl; R3, R4, and R5 are H, halo, alkyl, alkoxy, CF3, carbalkoxy), which were prepared, exhibited diuretic activity. Benzodiazepinone derivative II was heated with POCl3, and the 2,7-dichloro compound obtained was heated with 2,6-Me2C6H3NH2 at 140° to give I (R = Cl, R1 = R2 = R5 = H, R3 = 2-Me, R4 = 6-Me).

IT 90835-01-1 90835-02-2 90835-03-3

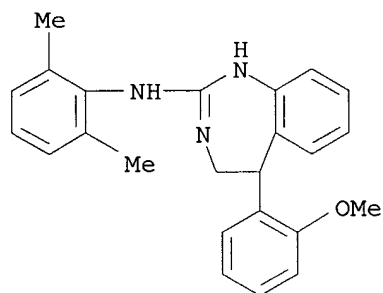
RL: RCT (Reactant); RACT (Reactant or reagent)
(anilinobenzodiazepines)

RN 90835-01-1 CAPLUS

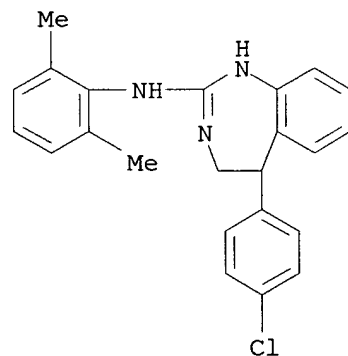
CN 1H-1,3-Benzodiazepin-2-amine, N-(2,6-dimethylphenyl)-4,5-dihydro-5-phenyl-
(9CI) (CA INDEX NAME)



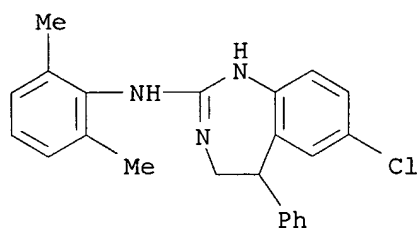
RN 90835-02-2 CAPLUS
 CN 1H-1,3-Benzodiazepin-2-amine, N-(2,6-dimethylphenyl)-4,5-dihydro-5-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 90835-03-3 CAPLUS
 CN 1H-1,3-Benzodiazepin-2-amine, 5-(4-chlorophenyl)-N-(2,6-dimethylphenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)

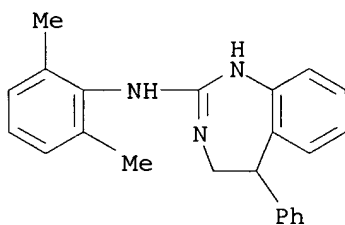


IT 90834-69-8P 90834-72-3P 90834-78-9P
 90834-83-6P 90834-85-8P 90834-89-2P
 90834-99-4P 90835-00-0P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and diuretic activity of)
 RN 90834-69-8 CAPLUS
 CN 1H-1,3-Benzodiazepin-2-amine, 7-chloro-N-(2,6-dimethylphenyl)-4,5-dihydro-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



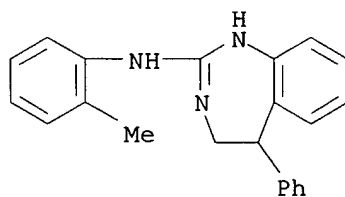
● HCl

RN 90834-72-3 CAPLUS
CN 1H-1,3-Benzodiazepin-2-amine, N-(2,6-dimethylphenyl)-4,5-dihydro-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

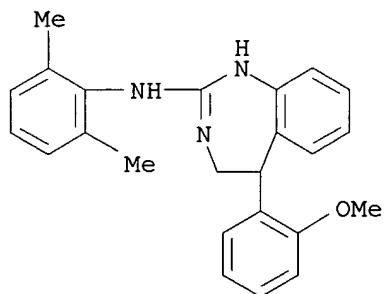
RN 90834-78-9 CAPLUS
CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-(2-methylphenyl)-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 90834-83-6 CAPLUS
CN 1H-1,3-Benzodiazepin-2-amine, N-(2,6-dimethylphenyl)-4,5-dihydro-5-(2-methoxyphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

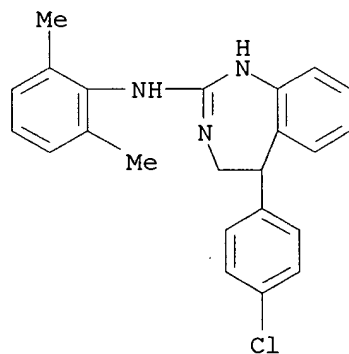
10/019,683



● HCl

RN 90834-85-8 CAPLUS

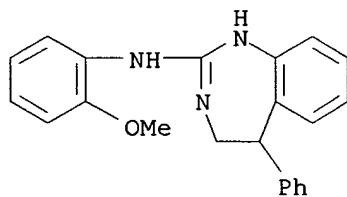
CN 1H-1,3-Benzodiazepin-2-amine, 5-(4-chlorophenyl)-N-(2,6-dimethylphenyl)-4,5-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 90834-89-2 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-(2-methoxyphenyl)-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

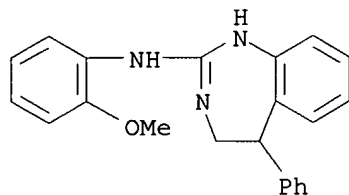


● HCl

10/019,683

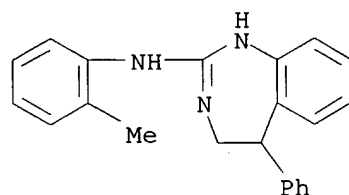
RN 90834-99-4 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-(2-methoxyphenyl)-5-phenyl-
(9CI) (CA INDEX NAME)



RN 90835-00-0 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-(2-methylphenyl)-5-phenyl-
(9CI) (CA INDEX NAME)

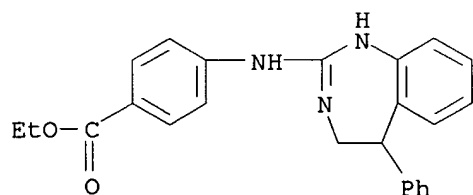


IT 90834-97-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and saponification of)

RN 90834-97-2 CAPLUS

CN Benzoic acid, 4-[(4,5-dihydro-5-phenyl-1H-1,3-benzodiazepin-2-yl)amino]-,
ethyl ester (9CI) (CA INDEX NAME)



IT 90834-71-2P 90834-73-4P 90834-74-5P

90834-75-6P 90834-76-7P 90834-77-8P

90834-79-0P 90834-80-3P 90834-81-4P

90834-82-5P 90834-84-7P 90834-86-9P

90834-87-0P 90834-88-1P 90834-90-5P

90834-91-6P 90834-92-7P 90834-93-8P

90834-95-0P 90834-96-1P 90834-98-3P

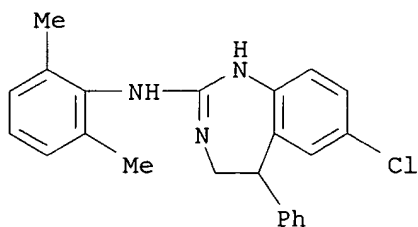
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 90834-71-2 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, 7-chloro-N-(2,6-dimethylphenyl)-4,5-dihydro-

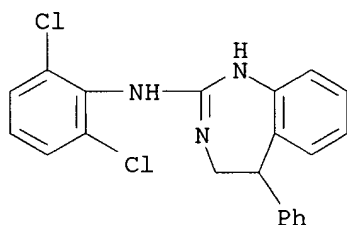
10/019,683

5-phenyl- (9CI) (CA INDEX NAME)



RN 90834-73-4 CAPLUS

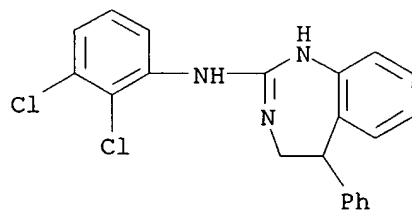
CN 1H-1,3-Benzodiazepin-2-amine, N-(2,6-dichlorophenyl)-4,5-dihydro-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 90834-74-5 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, N-(2,3-dichlorophenyl)-4,5-dihydro-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

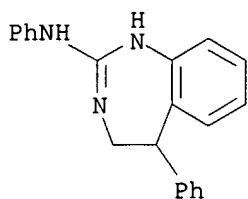


RN 90834-75-6 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N,5-diphenyl- (9CI) (CA INDEX NAME)

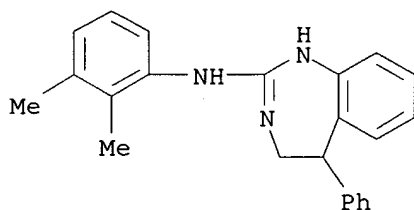


10/019,683



RN 90834-76-7 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, N-(2,3-dimethylphenyl)-4,5-dihydro-5-phenyl-
(9CI) (CA INDEX NAME)



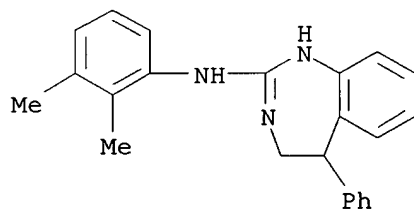
RN 90834-77-8 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, N-(2,3-dimethylphenyl)-4,5-dihydro-5-phenyl-
, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 90834-76-7

CMF C23 H23 N3

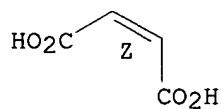


CM 2

CRN 110-16-7

CMF C4 H4 O4

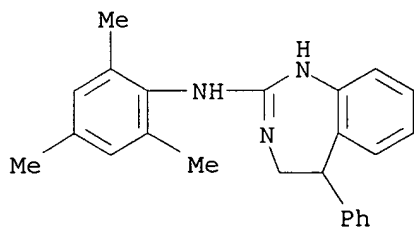
Double bond geometry as shown.



RN 90834-79-0 CAPLUS

10/019,683

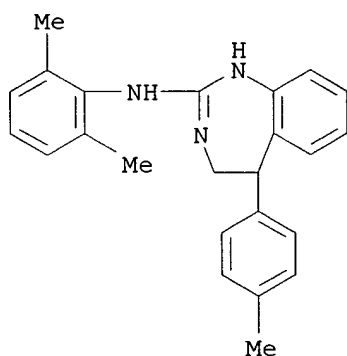
CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-5-phenyl-N-(2,4,6-trimethylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 90834-80-3 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, N-(2,6-dimethylphenyl)-4,5-dihydro-5-(4-methylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

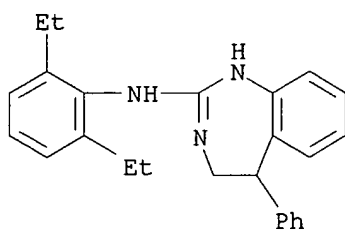


● HCl

RN 90834-81-4 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, N-(2,6-diethylphenyl)-4,5-dihydro-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

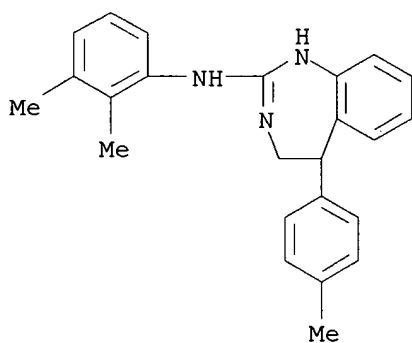
10/019,683



● HCl

RN 90834-82-5 CAPLUS

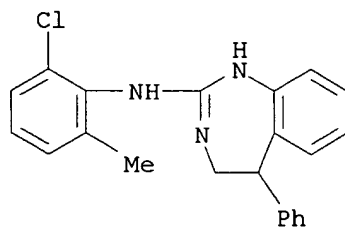
CN 1H-1,3-Benzodiazepin-2-amine, N-(2,3-dimethylphenyl)-4,5-dihydro-5-(4-methylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 90834-84-7 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, N-(2-chloro-6-methylphenyl)-4,5-dihydro-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

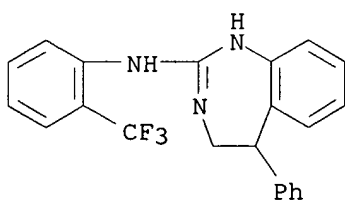


● HCl

RN 90834-86-9 CAPLUS

10/019,683

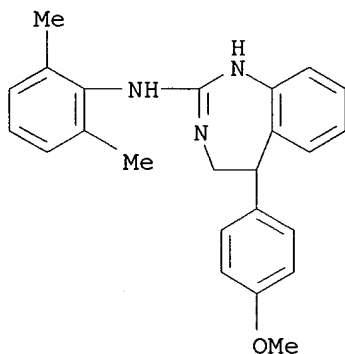
RN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-5-phenyl-N-[2-(trifluoromethyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 90834-87-0 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, N-(2,6-dimethylphenyl)-4,5-dihydro-5-(4-methoxyphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

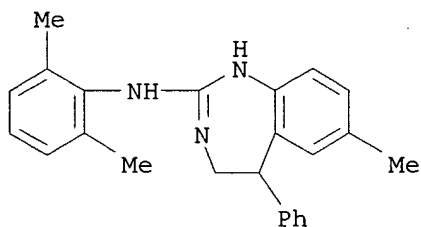


● HCl

RN 90834-88-1 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, N-(2,6-dimethylphenyl)-4,5-dihydro-7-methyl-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

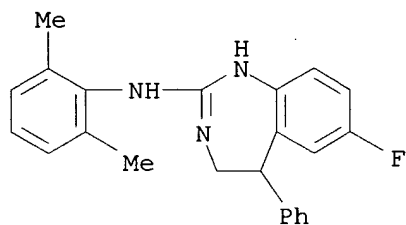
10/019,683



● HCl

RN 90834-90-5 CAPLUS

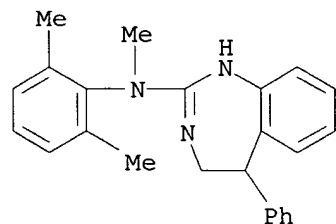
CN 1H-1,3-Benzodiazepin-2-amine, N-(2,6-dimethylphenyl)-7-fluoro-4,5-dihydro-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 90834-91-6 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, N-(2,6-dimethylphenyl)-4,5-dihydro-N-methyl-5-phenyl- (9CI) (CA INDEX NAME)



RN 90834-92-7 CAPLUS

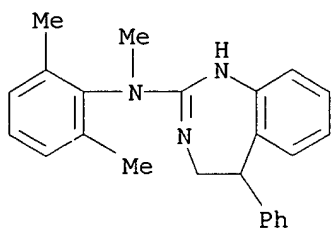
CN 1H-1,3-Benzodiazepin-2-amine, N-(2,6-dimethylphenyl)-4,5-dihydro-N-methyl-5-phenyl-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 90834-91-6

CMF C24 H25 N3

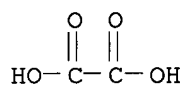
10/019,683



CM 2

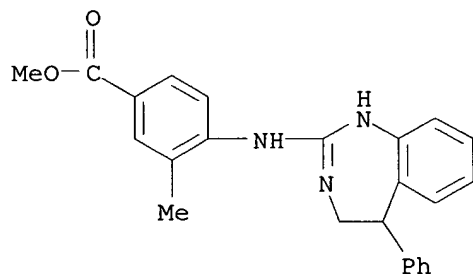
CRN 144-62-7

CMF C2 H2 O4



RN 90834-93-8 CAPLUS

CN Benzoic acid, 4-[(4,5-dihydro-5-phenyl-1H-1,3-benzodiazepin-2-yl)amino]-3-methyl-, methyl ester (9CI) (CA INDEX NAME)



RN 90834-95-0 CAPLUS

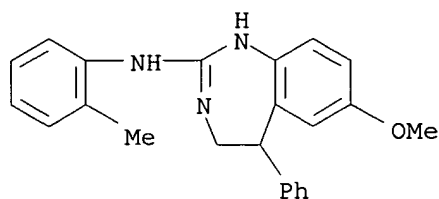
CN Ethanedioic acid, monoethyl ester, compd. with 4,5-dihydro-7-methoxy-N-(2-methylphenyl)-5-phenyl-1H-1,3-benzodiazepin-2-amine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 90834-94-9

CMF C23 H23 N3 O

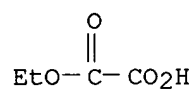
10/019,683



CM 2

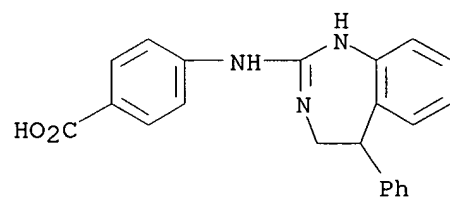
CRN 617-37-8

CMF C4 H6 O4



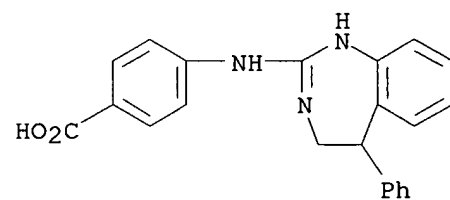
RN 90834-96-1 CAPLUS

CN Benzoic acid, 4-[(4,5-dihydro-5-phenyl-1H-1,3-benzodiazepin-2-yl)amino]-
(9CI) (CA INDEX NAME)



RN 90834-98-3 CAPLUS

CN Benzoic acid, 4-[(4,5-dihydro-5-phenyl-1H-1,3-benzodiazepin-2-yl)amino]-,
monohydrochloride (9CI) (CA INDEX NAME)



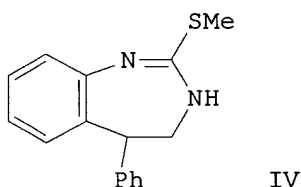
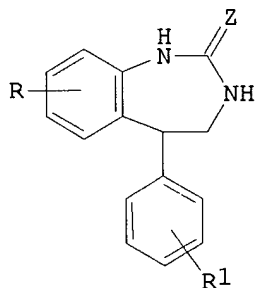
● HCl

L14 ANSWER 30 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:209887 CAPLUS
 DOCUMENT NUMBER: 100:209887
 TITLE: 5-Phenyl-1,3-benzodiazepines and intermediates
 INVENTOR(S): Bayssat, Michel; Ferrand, Gerard
 PATENT ASSIGNEE(S): LIPHA, Lyonnaise Industrielle Pharmaceutique, Fr.
 SOURCE: Fr. Demande, 19 pp.
 CODEN: FRXXBL
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--|----------|-----------------|----------|
| FR 2528838 | A1 | 19831223 | FR 1982-10466 | 19820616 |
| FR 2528838 | B1 | 19851011 | | |
| PRIORITY APPLN. INFO.: | | | FR 1982-10466 | 19820616 |
| OTHER SOURCE(S): | CASREACT 100:209887; MARPAT 100:209887 | | | |

GI



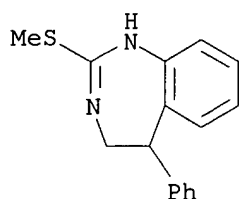
AB Benzodiazepines I (Z = O, S; R and R1 are H, halo, alkyl, alkoxy), useful as intermediates, especially for pharmaceuticals, were prepared. Thus, 2-H₂NC₆H₄CHPhCH₂NH₂ (II) was treated with CS₂ to give I (Z = S, R = R1 = H) (III). The cyclocondensation of II with 1,1'-carbonyldiimidazole gave I (Z = O, R = R1 = H), which was also prepared by the H₂O₂ oxidation of sulfide IV.

IT 90141-77-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to base)

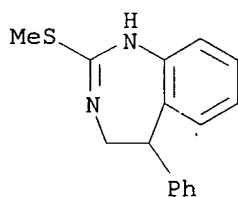
RN 90141-77-8 CAPLUS

CN 3H-1,3-Benzodiazepine, 4,5-dihydro-2-(methylthio)-5-phenyl-,
monohydriodide (9CI) (CA INDEX NAME)

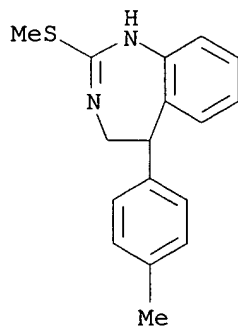


● HI

IT 90141-78-9P 90156-43-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and hydrolysis of, benzodiazepinone from)
 RN 90141-78-9 CAPLUS
 CN 3H-1,3-Benzodiazepine, 4,5-dihydro-2-(methylthio)-5-phenyl- (9CI) (CA
 INDEX NAME)



RN 90156-43-7 CAPLUS
 CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-(4-methylphenyl)-2-(methylthio)-,
 monohydriodide (9CI) (CA INDEX NAME)



● HI

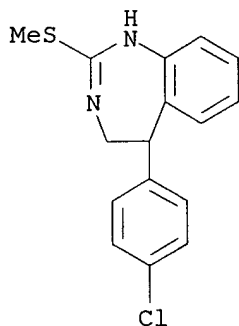
IT 90156-45-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

10/019,683

(preparation and hydrolysis of, benzodiazepone from)

RN 90156-45-9 CAPLUS

CN 1H-1,3-Benzodiazepine, 5-(4-chlorophenyl)-4,5-dihydro-2-(methylthio)-, monohydriodide (9CI) (CA INDEX NAME)



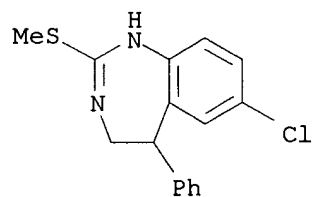
● HI

IT 90156-41-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 90156-41-5 CAPLUS

CN 1H-1,3-Benzodiazepine, 7-chloro-4,5-dihydro-2-(methylthio)-5-phenyl-, monohydriodide (9CI) (CA INDEX NAME)



● HI

10/019,683

L14 ANSWER 31 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:103402 CAPLUS

DOCUMENT NUMBER: 100:103402

TITLE: Condensed 1,3-benzodiazepines and medicines containing them

INVENTOR(S): Ferrand, Gerard; Bayssat, Michel; Depin, Jean Claude; Betbeder-Matibet, Annie

PATENT ASSIGNEE(S): LIPHA, Lyonnaise Industrielle Pharmaceutique, Fr.

SOURCE: Fr. Demande, 15 pp.

CODEN: FRXXBL

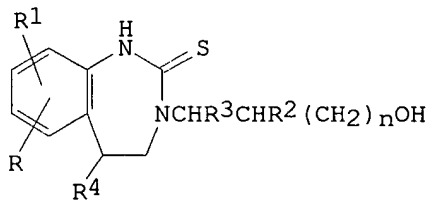
DOCUMENT TYPE: Patent

LANGUAGE: French

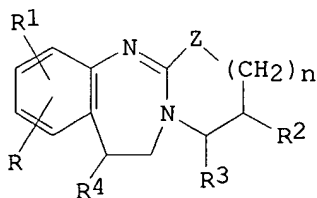
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|--|----------|
| FR 2521563 | A1 | 19830819 | FR 1982-2554 | 19820217 |
| FR 2521563 | B1 | 19840420 | | |
| PRIORITY APPLN. INFO.: | | | FR 1982-2554 | 19820217 |
| OTHER SOURCE(S): | | | CASREACT 100:103402; MARPAT 100:103402 | |
| GI | | | | |



I



II

AB Benzodiazepinethiones I ($n = 0, 1$; R and R1 are H, halo, alkoxy, OH, NO₂, NH₂; R₂ and R₃ are H, alkyl, Ph; R₄ = H, alkyl, Ph) were converted to fused compds. II ($Z = S, O$), which exhibited antidepressant activity. Thus, I ($n = 0, R = R_1 = R_2 = R_3 = R_4 = H$) (III) was heated with MeSO₃H at 100° to give II ($Z = S, n = 0, R = R_1 = R_2 = R_3 = R_4 = H$) (IV). A mixture of III and MeI in EtOH was refluxed to give II ($Z = O, n = 0, R = R_1 = R_2 = R_3 = R_4 = H$) hydriodide. IV. HCl inhibited reserpine-induced ptosis in mice with an ED₅₀ value smaller than that of imipramine.

IT 88519-17-9P 88519-19-1P 88519-25-9P

88519-30-6P 88519-34-0P 88519-41-9P

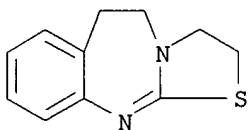
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and antidepressant activity of)

RN 88519-17-9 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-, monohydrochloride

10/019,683

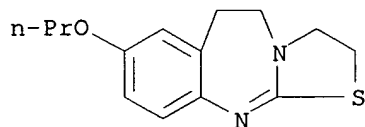
(9CI) (CA INDEX NAME)



● HCl

RN 88519-19-1 CAPLUS

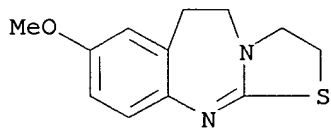
CN Thiazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-8-propoxy-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 88519-25-9 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-8-methoxy-,
monohydrochloride (9CI) (CA INDEX NAME)

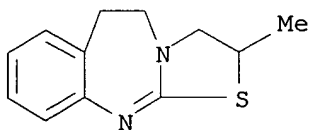


● HCl

RN 88519-30-6 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-2-methyl-,
monohydrochloride (9CI) (CA INDEX NAME)

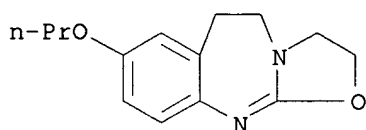
10/019,683



● HCl

RN 88519-34-0 CAPLUS

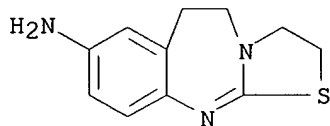
CN Oxazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-8-propoxy-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 88519-41-9 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepin-8-amine, 2,3,5,6-tetrahydro-,
dihydrochloride (9CI) (CA INDEX NAME)



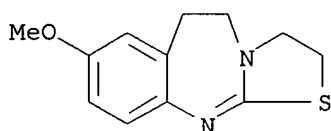
●2 HCl

IT 88519-36-2P

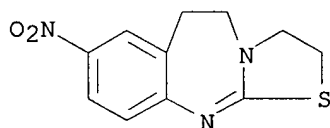
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and demethylation of)

RN 88519-36-2 CAPLUS

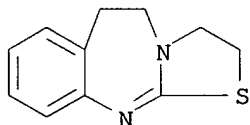
CN Thiazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-8-methoxy- (9CI)
(CA INDEX NAME)



IT 88519-40-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reduction of)
 RN 88519-40-8 CAPLUS
 CN Thiazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-8-nitro- (9CI) (CA
 INDEX NAME)

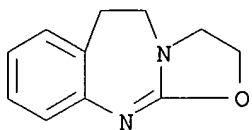


IT 88519-18-0P 88519-20-4P 88519-21-5P
 88519-22-6P 88519-23-7P 88519-24-8P
 88519-26-0P 88519-27-1P 88519-28-2P
 88519-31-7P 88519-32-8P 88519-33-9P
 88519-35-1P 88519-37-3P 88519-38-4P
 88519-39-5P 88519-42-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 88519-18-0 CAPLUS
 CN Thiazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro- (9CI) (CA INDEX
 NAME)



RN 88519-20-4 CAPLUS
 CN Oxazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-, monohydrochloride
 (9CI) (CA INDEX NAME)

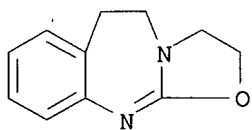
10/019,683



● HCl

RN 88519-21-5 CAPLUS

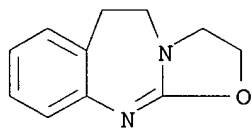
CN Oxazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-, monohydriodide (9CI) (CA INDEX NAME)



● HI

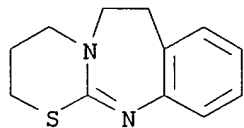
RN 88519-22-6 CAPLUS

CN Oxazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro- (9CI) (CA INDEX NAME)



RN 88519-23-7 CAPLUS

CN 2H-[1,3]Thiazino[2,3-b][1,3]benzodiazepine, 3,4,6,7-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)



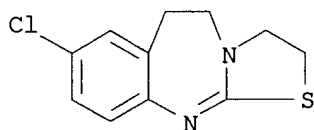
● HCl

RN 88519-24-8 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 8-chloro-2,3,5,6-tetrahydro-,

10/019,683

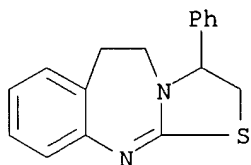
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 88519-26-0 CAPLUS

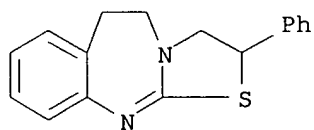
CN Thiazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-3-phenyl-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 88519-27-1 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-2-phenyl-,
monohydrochloride (9CI) (CA INDEX NAME)

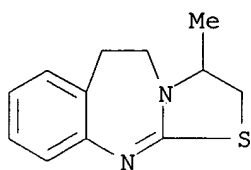


● HCl

RN 88519-28-2 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-3-methyl-,
monohydrochloride (9CI) (CA INDEX NAME)

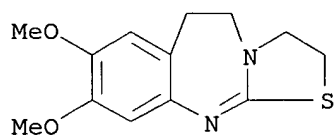
10/019,683



● HCl

RN 88519-31-7 CAPLUS

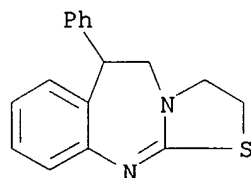
CN Thiazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-8,9-dimethoxy-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 88519-32-8 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-6-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

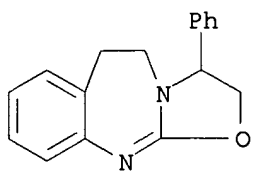


● HCl

RN 88519-33-9 CAPLUS

CN Oxazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-3-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

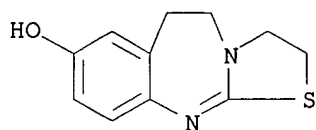
10/019,683



● HCl

RN 88519-35-1 CAPLUS

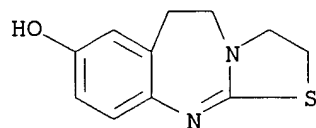
CN Thiazolo[2,3-b][1,3]benzodiazepin-8-ol, 2,3,5,6-tetrahydro-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 88519-37-3 CAPLUS

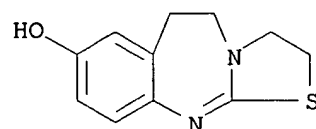
CN Thiazolo[2,3-b][1,3]benzodiazepin-8-ol, 2,3,5,6-tetrahydro-,
monohydrobromide (9CI) (CA INDEX NAME)



● HBr

RN 88519-38-4 CAPLUS

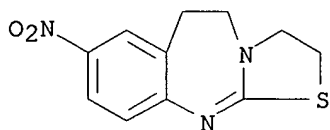
CN Thiazolo[2,3-b][1,3]benzodiazepin-8-ol, 2,3,5,6-tetrahydro- (9CI) (CA
INDEX NAME)



RN 88519-39-5 CAPLUS

10/019,683

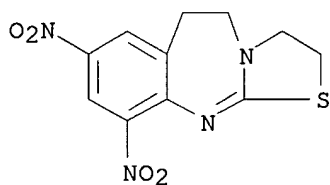
CN Thiazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-8-nitro-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 88519-42-0 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-8,10-dinitro- (9CI)
(CA INDEX NAME)



L14 ANSWER 32 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:85663 CAPLUS

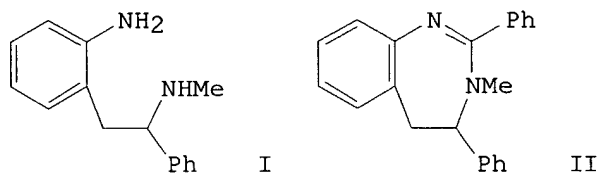
DOCUMENT NUMBER: 100:85663

TITLE: (\pm)-4-Aryl-4,5-dihydro-3H-1,3-benzodiazepines. 3.
2-Phenyl and 2-amino analogs as potential
antihypertensive agentsAUTHOR(S): Setescak, Linda L.; Dekow, Frederick W.; Kitzen, Jan
M.; Martin, Lawrence L.CORPORATE SOURCE: Dep. Chem. Res., Hoechst-Roussel Pharm., Inc.,
Somerville, NJ, 08876, USASOURCE: Journal of Medicinal Chemistry (1984), 27(3), 401-4
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



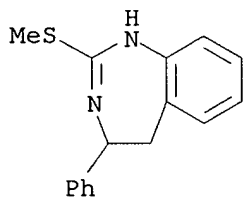
AB A series of 2-phenyl- and 2-amino-4-aryl-4,5-dihydro-3H-1,3-benzodiazepines was prepared by cyclization of diamines, e.g. I, with orthoesters and submitted for broad biol. screening, including evaluation for potential antihypertensive activity. (\pm)-4,5-Dihydro-2,4-diphenyl-3-methyl-3H-1,3-benzodiazepine hydrochloride (II) was the most active member of the series in the spontaneously hypertensive rat model, producing a 56-mm decrease in systolic blood pressure at 50 mg/kg orally. The synthesis of II analogs containing nuclear substituents in the 4-Ph moiety resulted in a marked decrease of antihypertensive activity. It was not possible to improve on the antihypertensive properties of II through further synthetic modifications.

IT 88057-63-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antihypertensive activity of)

RN 88057-63-0 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(methylthio)-4-phenyl- (9CI) (CA
INDEX NAME)



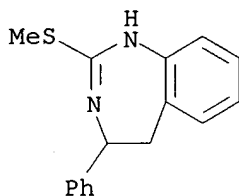
10/019,683

IT 88057-51-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reaction with methylpiperazine or morpholine and
antihypertensive activity of)

RN 88057-51-6 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(methylthio)-4-phenyl-,
monohydriodide (9CI) (CA INDEX NAME)



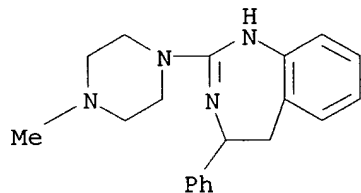
● HI

IT 88057-52-7P 88057-53-8P 88057-55-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

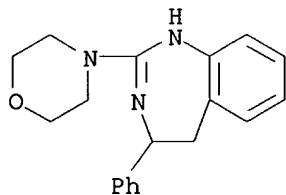
RN 88057-52-7 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(4-methyl-1-piperazinyl)-4-phenyl-
(9CI) (CA INDEX NAME)



RN 88057-53-8 CAPLUS

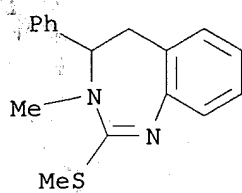
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(4-morpholinyl)-4-phenyl- (9CI) (CA
INDEX NAME)



RN 88057-55-0 CAPLUS

CN 3H-1,3-Benzodiazepine, 4,5-dihydro-3-methyl-2-(methylthio)-4-phenyl-,
monohydriodide (9CI) (CA INDEX NAME)

10/019,683



● HI

~~114~~ ANSWER 33 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:558476 CAPLUS

DOCUMENT NUMBER: 99:158476

TITLE: Imidazobenzodiazepines, pharmaceutical preparations containing these compounds and their therapeutic use

INVENTOR(S): Vlattas, Isidoros

PATENT ASSIGNEE(S): Ciba-Geigy A.-G. , Switz.

SOURCE: Eur. Pat. Appl., 56 pp.

CODEN: EPXXDW

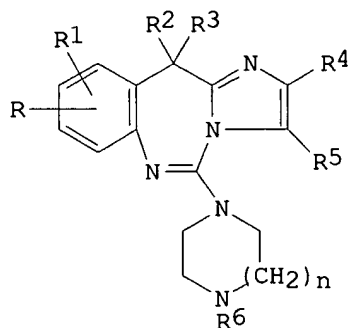
DOCUMENT TYPE: Patent

LANGUAGE: German

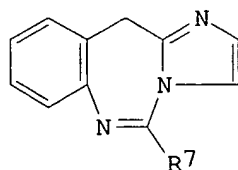
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|--------------------------------------|----------|-----------------|------------|
| EP 81461 | A2 | 19830615 | EP 1982-810516 | 19821201 |
| EP 81461 | A3 | 19840718 | | |
| R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE | | | | |
| US 4459232 | A | 19840710 | US 1982-417746 | 19820913 |
| US 4460508 | A | 19840717 | US 1982-417747 | 19820913 |
| FI 8204170 | A | 19830608 | FI 1982-4170 | 19821103 |
| GB 2115407 | A1 | 19830907 | GB 1982-34334 | 19821202 |
| GB 2115407 | B2 | 19850724 | | |
| ES 517912 | A1 | 19841201 | ES 1982-517912 | 19821203 |
| CA 1180011 | A1 | 19841225 | CA 1982-416953 | 19821203 |
| DK 8205402 | A | 19830608 | DK 1982-5402 | 19821206 |
| NO 8204090 | A | 19830608 | NO 1982-4090 | 19821206 |
| AU 8291315 | A1 | 19830616 | AU 1982-91315 | 19821206 |
| JP 58109489 | A2 | 19830629 | JP 1982-212828 | 19821206 |
| ZA 8208954 | A | 19830928 | ZA 1982-8954 | 19821206 |
| DD 203547 | A5 | 19831026 | DD 1982-245615 | 19821206 |
| HU 27368 | O | 19831028 | HU 1982-3911 | 19821206 |
| HU 187191 | B | 19851128 | | |
| ES 530125 | A1 | 19851101 | ES 1984-530125 | 19840228 |
| PRIORITY APPLN. INFO.: | | | US 1981-328274 | A 19811207 |
| OTHER SOURCE(S): | CASREACT 99:158476; MARPAT 99:158476 | | | |
| GI | | | | |



I



II

AB The title compds. (I; R, R1, R4-R6 = H, alkyl, alkenyl, alkanoyl, halo,

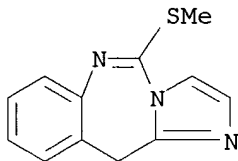
cyano, alkoxy carbonyl, alkylthio, sulfamoyl, etc.; R₂, R₃ = H, alkyl, n = 1, 2) and their oxides and quaternary derivs. were prepared. Thus, 2-MeC₆H₄NO₂ was condensed with (CO₂Et)₂ and treated with HONH₂.HCl to give 2-O₂NC₆H₄CH₂C(:NOH)CO₂Et. This was saponified, decarboxylated, and dehydrated to give 2-O₂NC₆H₄CH₂CN, which was treated with EtOH to give 2-O₂NC₆H₄CH₂C(:NH)CO₂Et. This was cyclocondensed with H₂NCH₂CH(OMe)₂ to give 2-(2-nitrobenzyl)-1H-imidazole, which was treated with CSCl₂ and methylated to give II (R₇ = MeS). This was condensed with 1-methylpiperazine to give II (R₇ = 4-methyl-1-piperazinyl). I are effective tranquilizers at 10-30 mg/kg orally.

IT 87081-83-2P 87081-92-3P 87081-98-9P
87082-08-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation of, with piperazine)

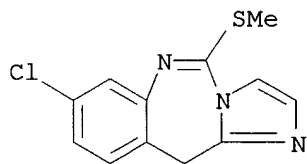
RN 87081-83-2 CAPLUS

CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(methylthio)- (9CI) (CA INDEX NAME)



RN 87081-92-3 CAPLUS

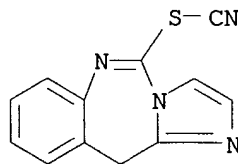
CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 8-chloro-5-(methylthio)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 87081-98-9 CAPLUS

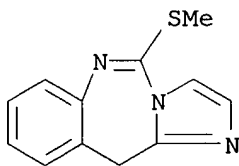
CN Thiocyanic acid, 11H-imidazo[1,2-c][1,3]benzodiazepin-5-yl ester (9CI)
(CA INDEX NAME)



RN 87082-08-4 CAPLUS

10/019,683

CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(methylthio)-, hydrochloride
(9CI) (CA INDEX NAME)



●x HCl

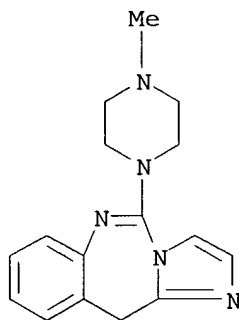
IT 87081-84-3P 87081-85-4P 87082-04-0P

87082-05-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and tranquilizer activity of)

RN 87081-84-3 CAPLUS

CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(4-methyl-1-piperazinyl)- (9CI)
(CA INDEX NAME)



RN 87081-85-4 CAPLUS

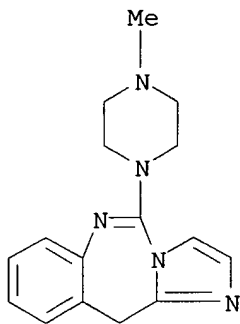
CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(4-methyl-1-piperazinyl)-,
(2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 87081-84-3

CMF C16 H19 N5

10/019,683

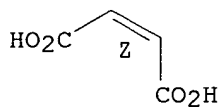


CM 2

CRN 110-16-7

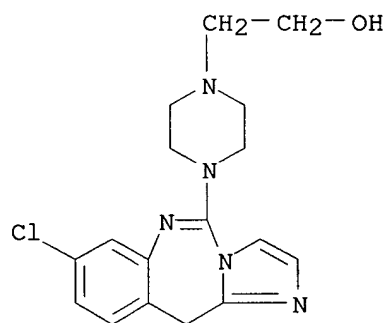
CMF C4 H4 O4

Double bond geometry as shown.



RN 87082-04-0 CAPLUS

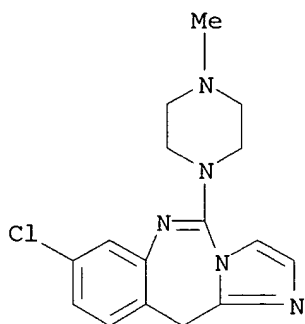
CN 1-Piperazineethanol, 4-(8-chloro-11H-imidazo[1,2-c][1,3]benzodiazepin-5-yl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

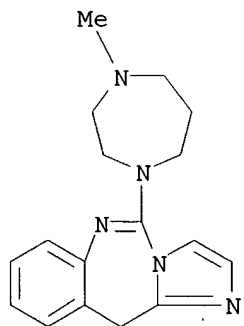
RN 87082-05-1 CAPLUS

CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 8-chloro-5-(4-methyl-1-piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)



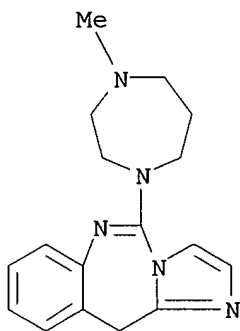
●2 HCl

IT 87081-94-5P 87081-95-6P 87082-00-6P
 87082-03-9P 87082-06-2P 87082-07-3P
 87082-09-5P 87082-10-8P 87082-11-9P
 87082-12-0P 87082-14-2P 87082-17-5P
 87092-49-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 87081-94-5 CAPLUS
 CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(hexahydro-4-methyl-1H-1,4-
 diazepin-1-yl)- (9CI) (CA INDEX NAME)



RN 87081-95-6 CAPLUS
 CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(hexahydro-4-methyl-1H-1,4-
 diazepin-1-yl)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)
 CM 1
 CRN 87081-94-5
 CMF C17 H21 N5

10/019,683

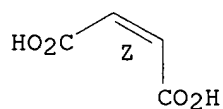


CM 2

CRN 110-16-7

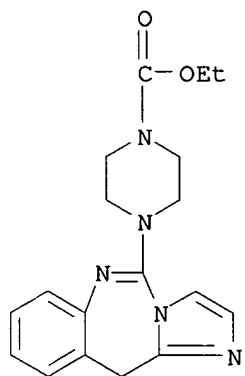
CMF C4 H4 O4

Double bond geometry as shown.



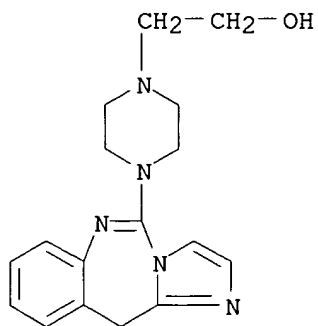
RN 87082-00-6 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-(11H-imidazo[1,2-c][1,3]benzodiazepine-5-yl)-, ethyl ester (9CI) (CA INDEX NAME)

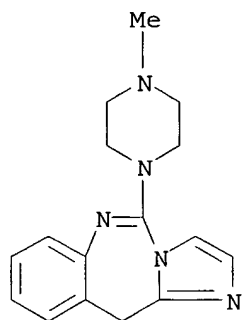


RN 87082-03-9 CAPLUS

CN 1-Piperazineethanol, 4-(11H-imidazo[1,2-c][1,3]benzodiazepine-5-yl)- (9CI) (CA INDEX NAME)



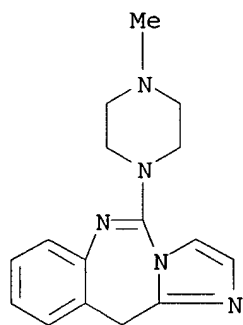
RN 87082-06-2 CAPLUS
 CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(4-methyl-1-piperazinyl)-,
 dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

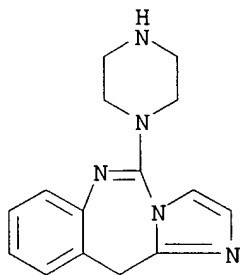
RN 87082-07-3 CAPLUS
 CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(4-methyl-1-piperazinyl)-,
 monohydrochloride (9CI) (CA INDEX NAME)

10/019,683

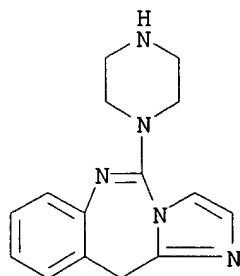


● HCl

RN 87082-09-5 CAPLUS
CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(1-piperazinyl)- (9CI) (CA INDEX NAME)



RN 87082-10-8 CAPLUS
CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(1-piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 87082-11-9 CAPLUS

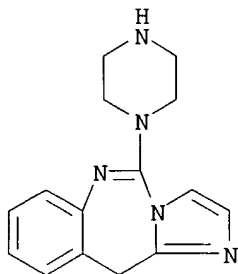
10/019,683

CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(1-piperazinyl)-,
(2Z)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 87082-09-5

CMF C15 H17 N5

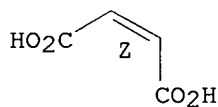


CM 2

CRN 110-16-7

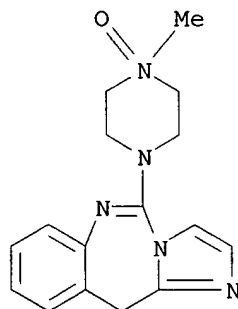
CMF C4 H4 O4

Double bond geometry as shown.



RN 87082-12-0 CAPLUS

CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(4-methyl-4-oxido-1-piperazinyl)-,
, hydrochloride (9CI) (CA INDEX NAME)

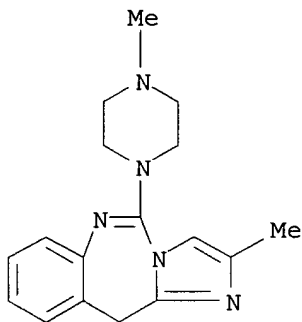


●x HCl

RN 87082-14-2 CAPLUS

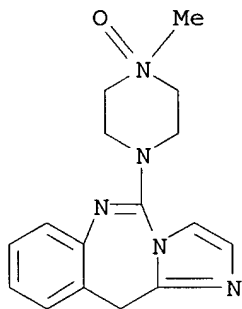
10/019,683

CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 2-methyl-5-(4-methyl-1-piperazinyl)-
(9CI) (CA INDEX NAME)



RN 87082-17-5 CAPLUS

CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 5-(4-methyl-4-oxido-1-piperazinyl)-
(9CI) (CA INDEX NAME)



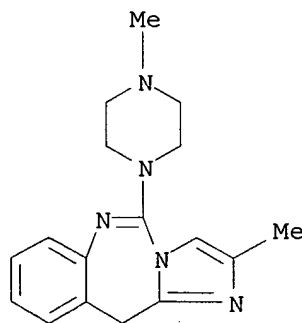
RN 87092-49-7 CAPLUS

CN 11H-Imidazo[1,2-c][1,3]benzodiazepine, 2-methyl-5-(4-methyl-1-piperazinyl)-
, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 87082-14-2

CMF C17 H21 N5



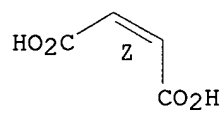
10/019,683

CM 2

CRN 110-16-7

CMF C4 H4 O4

Double bond geometry as shown.



10/019,683

~~LI~~ ANSWER 34 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:16653 CAPLUS

DOCUMENT NUMBER: 98:16653

TITLE: Cyclic guanidines

AUTHOR(S): Ognor, J. I.

CORPORATE SOURCE: Fac. Pharm., Univ. Benin, Benin City, Nigeria

SOURCE: Nigerian Journal of Pharmacy (1982), 13(3), 30-6

CODEN: NJPHDZ; ISSN: 0331-670X

DOCUMENT TYPE: Journal

LANGUAGE: English

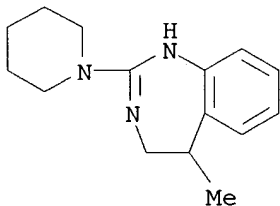
AB 4-RC6H4NHC(NR1R2):NCH2CH:CH2 (R = H, Me, Cl; NR1R2 = piperidino, morpholino, 4-methylpiperazino) were cyclized by polyphosphoric acid to give quinazoline and benzodiazepines and in a few cases 3,4-dihydroquinazolines.

IT 84006-85-9P 84006-86-0P 84006-92-8P
84006-93-9P 84006-94-0P 84006-95-1P
84007-01-2P 84007-02-3P 84007-03-4P
84007-04-5P 84007-12-5P 84007-13-6P
84007-16-9P 84007-17-0P 84007-20-5P
84007-21-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

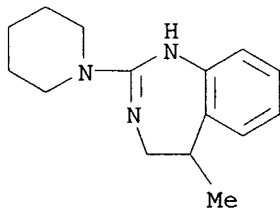
RN 84006-85-9 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-methyl-2-(1-piperidinyl)- (9CI) (CA INDEX NAME)



RN 84006-86-0 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-methyl-2-(1-piperidinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

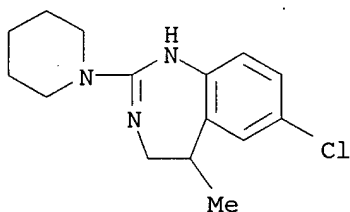


● HCl

RN 84006-92-8 CAPLUS

CN 1H-1,3-Benzodiazepine, 7-chloro-4,5-dihydro-5-methyl-2-(1-piperidinyl)- (9CI) (CA INDEX NAME)

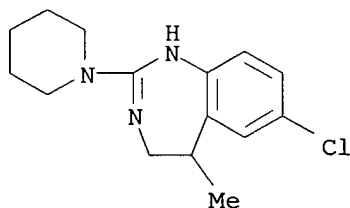
10/019,683



RN 84006-93-9 CAPLUS
CN Chromate(1-), diamminetetakis(thiocyanato-N)-, (OC-6-11)-, hydrogen, compd. with 7-chloro-4,5-dihydro-5-methyl-2-(1-piperidinyl)-1H-1,3-benzodiazepine (1:1) (9CI) (CA INDEX NAME)

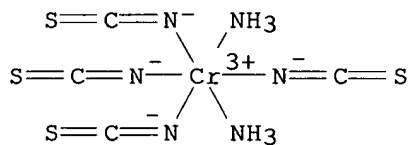
CM 1

CRN 84006-92-8
CMF C15 H20 Cl N3



CM 2

CRN 16925-04-5
CMF C4 H6 Cr N6 S4 . H
CCI CCS



● H⁺

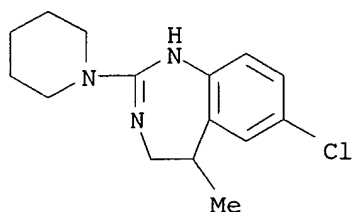
RN 84006-94-0 CAPLUS
CN 1H-1,3-Benzodiazepine, 7-chloro-4,5-dihydro-5-methyl-2-(1-piperidinyl)-, compd. with 2,4,6-trinitrophenol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 84006-92-8

10/019,683

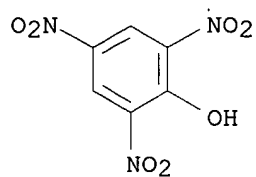
CMF C15 H20 Cl N3



CM 2

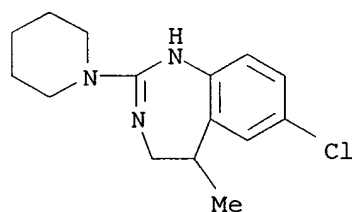
CRN 88-89-1

CMF C6 H3 N3 O7



RN 84006-95-1 CAPLUS

CN 1H-1,3-Benzodiazepine, 7-chloro-4,5-dihydro-5-methyl-2-(1-piperidinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

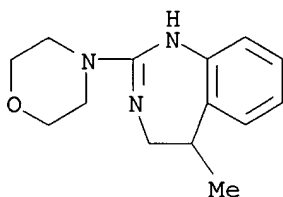


● HCl

RN 84007-01-2 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-methyl-2-(4-morpholinyl)- (9CI) (CA INDEX NAME)

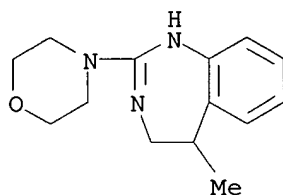
10/019,683



RN 84007-02-3 CAPLUS
CN Chromate(1-), diamminetetrakis(thiocyanato-N)-, (OC-6-11)-, hydrogen,
compd. with 4,5-dihydro-5-methyl-2-(4-morpholinyl)-1H-1,3-benzodiazepine
(1:1) (9CI) (CA INDEX NAME)

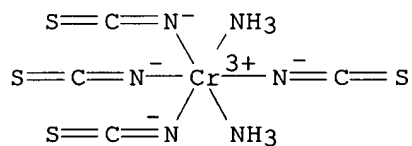
CM 1

CRN 84007-01-2
CMF C14 H19 N3 O



CM 2

CRN 16925-04-5
CMF C4 H6 Cr N6 S4 . H
CCI CCS



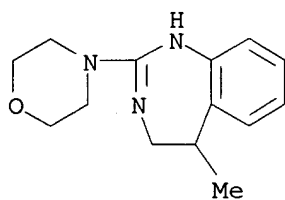
● H⁺

RN 84007-03-4 CAPLUS
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-methyl-2-(4-morpholinyl)-, compd.
with 2,4,6-trinitrophenol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 84007-01-2
CMF C14 H19 N3 O

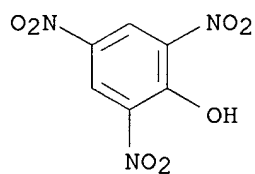
10/019,683



CM 2

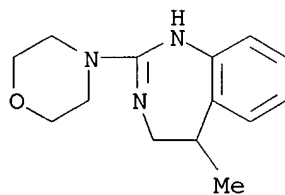
CRN 88-89-1

CMF C6 H3 N3 O7



RN 84007-04-5 CAPLUS

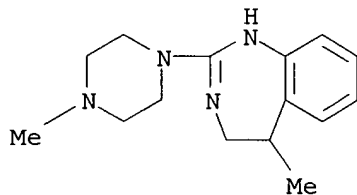
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-methyl-2-(4-morpholinyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 84007-12-5 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-methyl-2-(4-methyl-1-piperazinyl)-
(9CI) (CA INDEX NAME)



10/019,683

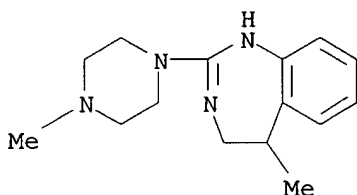
RN 84007-13-6 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5-methyl-2-(4-methyl-1-piperazinyl)-, compd. with 2,4,6-trinitrophenol (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 84007-12-5

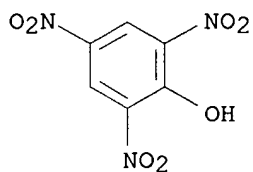
CMF C15 H22 N4



CM 2

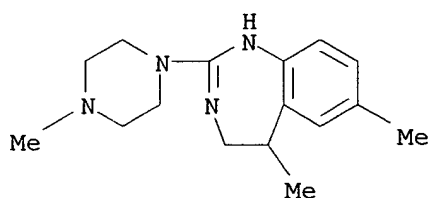
CRN 88-89-1

CMF C6 H3 N3 O7



RN 84007-16-9 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5,7-dimethyl-2-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



RN 84007-17-0 CAPLUS

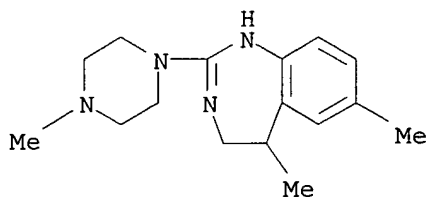
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-5,7-dimethyl-2-(4-methyl-1-piperazinyl)-, compd. with 2,4,6-trinitrophenol (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 84007-16-9

CMF C16 H24 N4

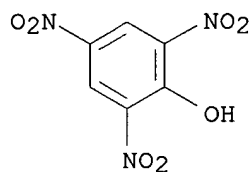
10/019,683



CM 2

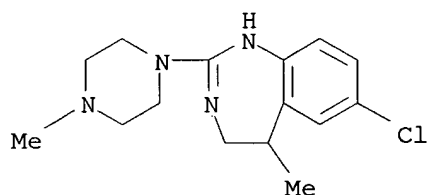
CRN 88-89-1

CMF C6 H3 N3 O7



RN 84007-20-5 CAPLUS

CN 1H-1,3-Benzodiazepine, 7-chloro-4,5-dihydro-5-methyl-2-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



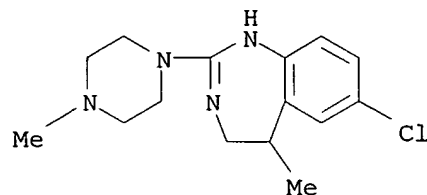
RN 84007-21-6 CAPLUS

CN 1H-1,3-Benzodiazepine, 7-chloro-4,5-dihydro-5-methyl-2-(4-methyl-1-piperazinyl)-, compd. with 2,4,6-trinitrophenol (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 84007-20-5

CMF C15 H21 Cl N4

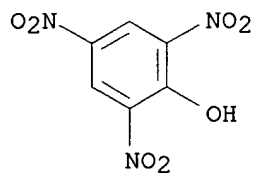


10/019,683

CM 2

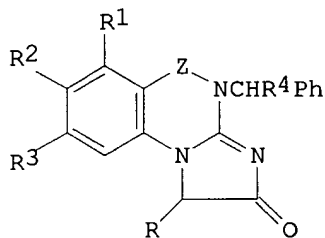
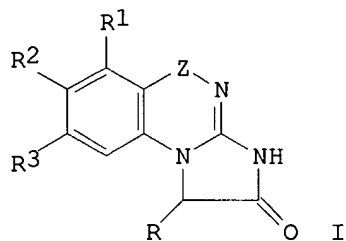
CRN 88-89-1

CMF C6 H3 N3 O7

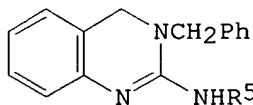


L14 ANSWER 35 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1981:532958 CAPLUS
 DOCUMENT NUMBER: 95:132958
 TITLE: Tricyclic compounds
 PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|------------|
| JP 56029591 | A2 | 19810324 | JP 1979-104818 | 19790817 |
| JP 62047186 | B4 | 19871006 | | |
| PRIORITY APPLN. INFO.: | | | JP 1979-104818 | A 19790817 |
| GI | | | | |



II



III

AB I (R = H, Me; R1 = H, Cl; R2 = H, Me, MeO; R3 = H, MeO; Z = CH2, CHMe, CH2CH2) or I.HCl were prepared by catalytic hydrogenation of II (R4 = H, Ph) or by heating II (R4 = Ph) with HCl in EtOH-H2O. Thus, 2.42 g III (R5 = H), 3.5 g Et3N, and 2.26 g ClCH2COCl in CHCl3 were stirred 1 h at room temperature to give III (R5 = COCH2Cl), which (1.26 g) was stirred with 0.56 g EtONa in EtOH for 2 h at room temperature to give II (R - R4 = H, Z = CH2)

(IV).

Hydrogenolysis of 1.20 g IV with concentrated HCl and 1.5 g 5% Pd-C in MeOH gave

I.HCl (R - R4 = H, Z = CH2). Some of I had blood platelet aggregation inhibiting activity with EC50 of 0.07-12.0 (collagen) and 5.8-82 (ADP).

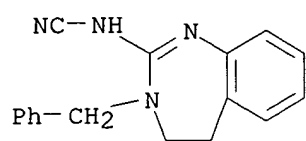
IT 75594-96-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

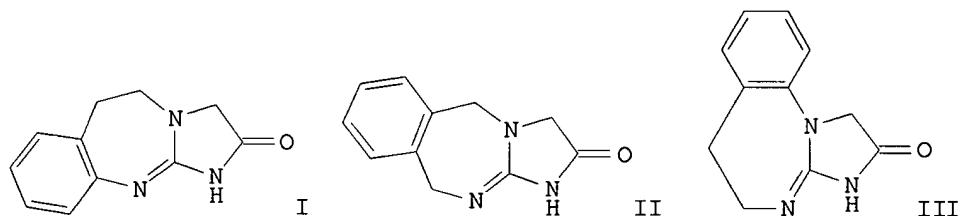
RN 75594-96-6 CAPLUS

CN Cyanamide, [4,5-dihydro-3-(phenylmethyl)-3H-1,3-benzodiazepin-2-yl]- (9CI)
 (CA INDEX NAME)

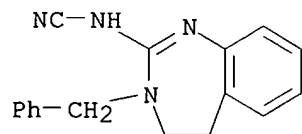
10/019,683



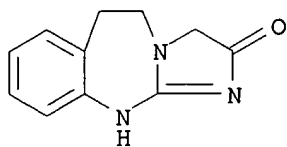
L14 ANSWER 36 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1980:620706 CAPLUS
 DOCUMENT NUMBER: 93:220706
 TITLE: Cyclic guanidines. VIII. Synthesis of imidazo-1,3-
 and -2,4-benzodiazepine derivatives as blood platelet
 aggregation inhibitors
 AUTHOR(S): Ishikawa, Fumiyoshi; Watanabe, Yoshifumi
 CORPORATE SOURCE: Res. Inst., Daiichi Seiyaku Co., Ltd., Tokyo, 132,
 Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1980), 28(4),
 1307-10
 CODEN: CPBTAL; ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Imidazo[2,1-b][1,3]- and -[2,4]benzodiazepin-2-ones I and II, and
 imidazo[1,2-a][1,3]benzodiazepin-2-one III were prepared as ring expansion
 analogs of a known aggregation inhibitor. III had potent activity, but I
 and II had little or no activity, resp.
 IT 75594-96-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and condensation of, with Et bromoacetate)
 RN 75594-96-6 CAPLUS
 CN Cyanamide, [4,5-dihydro-3-(phenylmethyl)-3H-1,3-benzodiazepin-2-yl]- (9CI)
 (CA INDEX NAME)

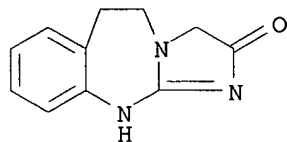


IT 75595-05-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 75595-05-0 CAPLUS
 CN 1H-Imidazo[2,1-b][1,3]benzodiazepin-2(3H)-one, 5,6-dihydro-,
 monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT 75594-94-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as blood platelet aggregation inhibitor)
RN 75594-94-4 CAPLUS
CN 1H-Imidazo[2,1-b][1,3]benzodiazepin-2(3H)-one, 5,6-dihydro- (9CI) (CA INDEX NAME)



~~101~~ ANSWER 37 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1980:198369 CAPLUS

DOCUMENT NUMBER: 92:198369

TITLE: Heterocyclic systems containing bridgehead nitrogen atom. XXXVI. Syntheses of dibenzo[d,f]1,3-diazepino[2,1:2',3']thiazolo[4',5'-b]quinoxaline, quinolino[3,2:5',4']thiazolo[3',2'-a]benzimidazole and 3-arylthiazolo[3,2-a]perimidine

AUTHOR(S): Gupta, V. K.; Sachdeva, M. L.; Dhaka, K. S.; Chadha, V. K.; Pujari, H. K.

CORPORATE SOURCE: Dep. Chem., Kurukshetra Univ., Kurukshetra, India

SOURCE: Annales de la Societe Scientifique de Bruxelles, Serie 1: Sciences Mathematiques, Astronomiques et Physiques (1979), 93(2), 137-41

CODEN: ASSBAH; ISSN: 0037-959X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 92:198369

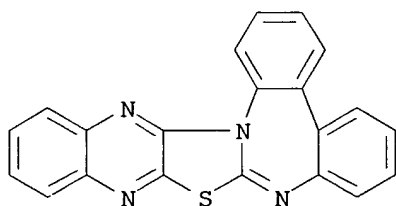
AB Dibenzo[df]-1,3-diazepino[2,1:2',3']thiazolo[4',5'-b]quinoxaline was prepared by treating 1H-dibenzo[d,f]-1,3-diazepine-2-thione with 2,3-dichloroquinoxaline. Quinolino[3,2:5',4']thiazolo[3',2'-a]benzimidazole was prepared by the condensation of thiazolo[3,2-a]benzimidazol-3(2H)-one with 2-O₂NC₆H₄CHO, followed by reductive cyclization. The reaction of 2-mercaptoperimidine with α -halo ketones and subsequent cyclization with polyphosphoric acid of the intermediate 2-arylmethylthioperimidines, yields 3-arylthiazolo[3,2-a]perimidines.

IT 73216-76-9P

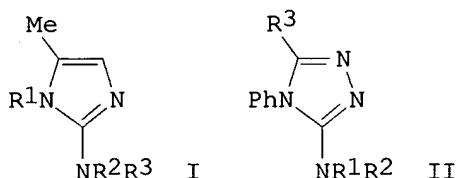
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 73216-76-9 CAPLUS

CN Dibenzo[4',5':6',7'] [1,3]diazepino[2',1':2,3]thiazolo[4,5-b]quinoxaline (9CI) (CA INDEX NAME)

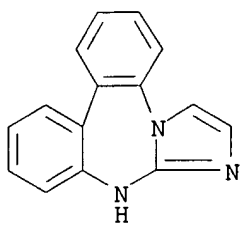


~~144~~ ANSWER 38 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1979:132750 CAPLUS
 DOCUMENT NUMBER: 90:132750
 TITLE: Synthesis and pharmacological study of
 2-aminoimidazoles and 3-amino-s-triazoles
 AUTHOR(S): Maffrand, Jean Pierre; Pereillo, Jean Marie; Eloy,
 Fernand; Aubert, Daniel; Rolland, Francoise;
 Barthelemy, Gerard
 CORPORATE SOURCE: Dep. Rech. Dev., PARCOPR, Toulouse, Fr.
 SOURCE: European Journal of Medicinal Chemistry (1978), 13(5),
 469-74
 CODEN: EJMCA5; ISSN: 0009-4374
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 GI



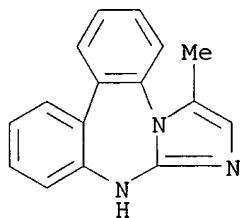
AB Twenty-three 2-amino-5-methylimidazoles (I; R1 = Me, allyl, Ph, or substituted Ph; R2 = H or Me, R3 = Ph or substituted Ph, or NR2R3 = N-containing heterocycle) were prepared by condensation of propargylamine [2450-71-7] with the appropriate isothioureas R1N=C(SMe)NR2R3 and spontaneous cyclization of the intermediate N-propargylguanidines. Similarly, sixteen 2-aminoimidazoles were prepared by condensation of the isothioureas with aminoacetaldehyde dimethylacetal [22483-09-6]. Ten isosteric 3-amino-s-triazoles (II; NR1R2 = diethylamino or N-containing heterocycle; R3 = Me or aryl) were prepared by condensation of PhN=C(SMe)NR1R2 with R3CONHNH2. Pharmacol. testing showed 4 I to have central nervous-stimulant activity. The most active was 5-methyl-1-phenyl-2-(1-pyrrolidinyl)imidazole (III) [57962-60-4], which was devoid of group toxicity in mice. III increased spontaneous motor activity, did not potentiate apomorphine-induced stereotyped behavior, and shortened barbiturate-induced sleeping times. III promoted escape activity in mice, did not produce tolerance in rats, and had sympathomimetic activity in dogs.
 IT 69584-20-9P 69584-21-0P
 RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
 (preparation and pharmacol. of)
 RN 69584-20-9 CAPLUS
 CN 8H-Dibenz[d,f]imidazo[1,2-a][1,3]diazepine (9CI) (CA INDEX NAME)

10/019,683



RN 69584-21-0 CAPLUS

CN 8H-Dibenz[d,f]imidazo[1,2-a][1,3]diazepine, 6-methyl- (9CI) (CA INDEX NAME)



10/019,683

LI4 ANSWER 39 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1977:171493 CAPLUS

DOCUMENT NUMBER: 86:171493

TITLE: 2-Amino-1-(2-bromo-3-substituted phenyl)pyridinium compounds

INVENTOR(S): Yale, Harry L.; Petigara, Ramesh B.

PATENT ASSIGNEE(S): E. R. Squibb and Sons, Inc., USA

SOURCE: U.S., 22 pp. Division of U.S. 3,957,787.

CODEN: USXXAM

DOCUMENT TYPE: Patent

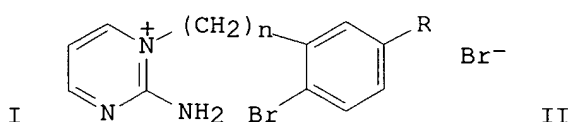
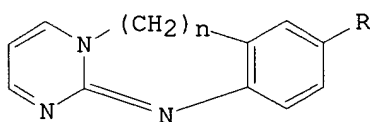
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| US 4001233 | A | 19770104 | US 1976-651390 | 19760122 |
| US 3868374 | A | 19750225 | US 1973-382804 | 19730726 |
| US 3957787 | A | 19760518 | US 1974-532796 | 19741216 |
| PRIORITY APPLN. INFO.: | | | US 1973-382804 | A3 19730726 |
| | | | US 1974-532796 | A3 19741216 |

GI



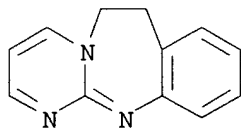
AB Pyrimido[2,1-b][1,3]benzodiazepine I (R = H, n = 2) and pyrimido[2,1-b][1,3]benzodiazocine I (R = MeS, n = 3) useful as central nervous system stimulants and muscle relaxants (no data), were prepared by cyclization of pyrimidinium bromides II. Thus, 9 g II (R = H, n = 2) in DMF was treated with 10.3 g K₂CO₃ and 0.5 g Cu bronze and the mixture heated 7 days at 100° to give 7.2 g I (R = H, n = 2). Refluxing a mixture of 212 g 2-BrC₆H₄CH₂CH₂Br and 121 g 2-aminopyrimidine in xylene for 3 h gave 170 g II (R = H, n = 2).

IT 56119-83-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 56119-83-6 CAPLUS

CN Pyrimido[2,1-b][1,3]benzodiazepine, 6,7-dihydro- (9CI) (CA INDEX NAME)



10/019,683

✓
LHA ANSWER 40 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1976:560142 CAPLUS

DOCUMENT NUMBER: 85:160142

TITLE: 1,2-Dihydro-2-imino-1-(bromophenylalkyl)pyrimidines

INVENTOR(S): Yale, Harry L.; Petigara, Ramesh B.

PATENT ASSIGNEE(S): E. R. Squibb and Sons, Inc., USA

SOURCE: U.S., 17 pp. Division of U.S. 3,868,374.

CODEN: USXXAM

DOCUMENT TYPE: Patent

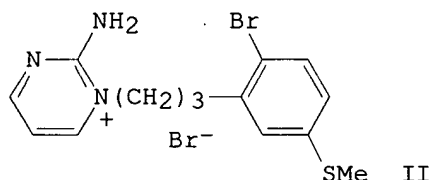
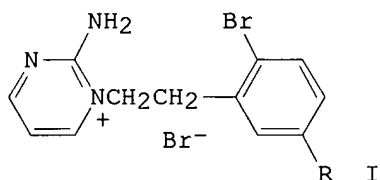
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| US 3957787 | A | 19760518 | US 1974-532796 | 19741216 |
| US 3868374 | A | 19750225 | US 1973-382804 | 19730726 |
| US 4001233 | A | 19770104 | US 1976-651390 | 19760122 |
| PRIORITY APPLN. INFO.: | | | US 1973-382804 | A3 19730726 |
| | | | US 1974-532796 | A3 19741216 |

GI



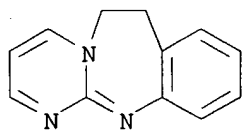
AB Phenethylpyrimidinium bromides I (R = H, Cl, SO₂NEt₂, SO₂NH₂, SO₂NPr₂) were prepared by brominating 2,5-Br(R)C₆H₃CH₂OH, treating 2,5-Br(R)C₆H₃CH₂Br with NaCN, ethanolysis of 2,5-Br(R)C₆H₃CH₂CN, reduction of 2,5-Br(R)C₆H₃CH₂CO₂Et, bromination of 2,5-Br(R)C₆H₃CH₂CH₂OH, and reaction of 2,5-Br(R)C₆H₃CH₂CH₂Br with 2-aminopyrimidine. I are bactericides with min. inhibitory concns. against Staphylococcus aureus of 3.13-12.5 γ/ml and are cyclized by Cu bronze-K₂CO₃ to pyrimidobenzodiazepines. The pyrimidinium salt II was similarly prepared and cyclized.

IT 56119-83-6P

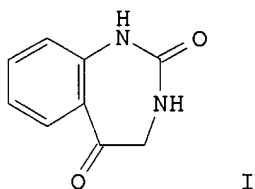
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 56119-83-6 CAPLUS

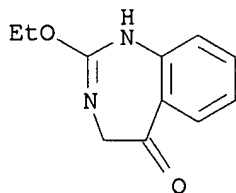
CN Pyrimido[2,1-b][1,3]benzodiazepine, 6,7-dihydro- (9CI) (CA INDEX NAME)



L14 ANSWER 41 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1976:508614 CAPLUS
 DOCUMENT NUMBER: 85:108614
 TITLE: Synthesis of some 1H-1,3-benzodiazepines
 AUTHOR(S): Taylor, John B.; Tully, W. Roger
 CORPORATE SOURCE: Roussel Lab. Ltd., Swindon, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 1: Organic and Bio-Organic Chemistry (1972-1999)
 (1976), (12), 1331-8
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 85:108614
 GI



AB 3,4-Dihydro-1H-1,3-benzodiazepine-2,5-dione (I) was prepared from o-nitroacetophenone. The critical step was the reaction of 2,2'-diaminoacetophenone with 1,1'-carbonyldiimidazole to give 77% N-(o-aminophenacylaminoacetyl)imidazole which cyclized readily in hot H₂O to give 88% I. The reactivity at positions 2, 5, and 7 was investigated. Attempts to introduce a 4,5-double bond resulted in rearrangement to quinolines and indoles.
 IT 60330-92-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reactions of)
 RN 60330-92-9 CAPLUS
 CN 5H-1,3-Benzodiazepin-5-one, 2-ethoxy-1,4-dihydro-, monohydrochloride (9CI)
 (CA INDEX NAME)



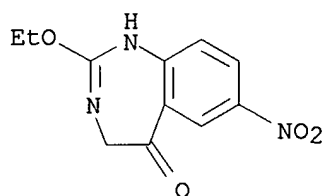
● HCl

IT 60330-97-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reduction of) ...

RN 60330-97-4 CAPLUS

CN 5H-1,3-Benzodiazepin-5-one, 2-ethoxy-1,4-dihydro-7-nitro- (9CI) (CA INDEX
NAME)

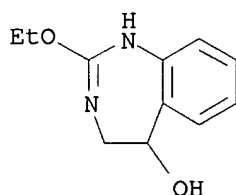


IT 60330-61-2P 60330-62-3P 60330-63-4P
60330-64-5P 60330-65-6P 60330-66-7P
60330-67-8P 60330-68-9P 60330-69-0P
60330-70-3P 60330-71-4P 60330-72-5P
60330-73-6P 60330-74-7P 60330-75-8P
60330-76-9P 60330-77-0P 60330-79-2P
60330-80-5P 60330-81-6P 60330-82-7P
60360-75-0P 60407-42-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 60330-61-2 CAPLUS

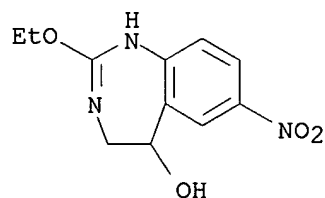
CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-4,5-dihydro-, monohydrochloride (9CI)
(CA INDEX NAME)



● HCl

RN 60330-62-3 CAPLUS

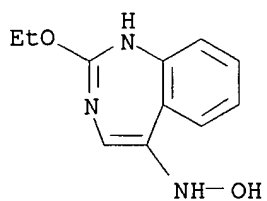
CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-4,5-dihydro-7-nitro- (9CI) (CA INDEX
NAME)



10/019,683

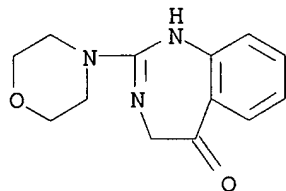
RN 60330-63-4 CAPLUS

CN 1H-1,3-Benzodiazepin-5-amine, 2-ethoxy-N-hydroxy- (9CI) (CA INDEX NAME)



RN 60330-64-5 CAPLUS

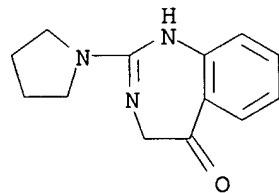
CN 5H-1,3-Benzodiazepin-5-one, 1,4-dihydro-2-(4-morpholinyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 60330-65-6 CAPLUS

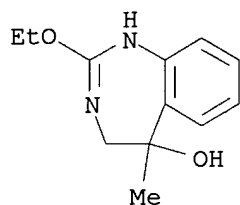
CN 5H-1,3-Benzodiazepin-5-one, 1,4-dihydro-2-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)



RN 60330-66-7 CAPLUS

CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-4,5-dihydro-5-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

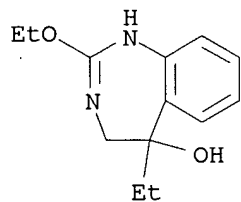




● HCl

RN 60330-67-8 CAPLUS

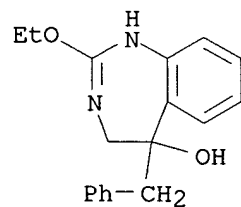
CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-5-ethyl-4,5-dihydro-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 60330-68-9 CAPLUS

CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-4,5-dihydro-5-(phenylmethyl)-,
monohydrochloride (9CI) (CA INDEX NAME)

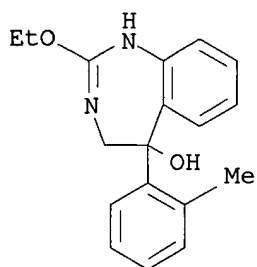


● HCl

RN 60330-69-0 CAPLUS

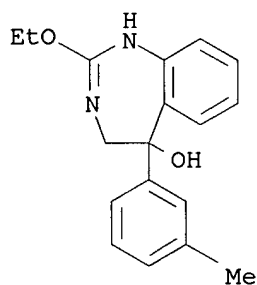
CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-4,5-dihydro-5-(2-methylphenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)

10/019,683



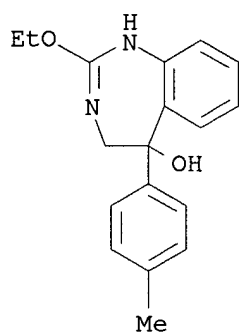
● HCl

RN 60330-70-3 CAPLUS
CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-4,5-dihydro-5-(3-methylphenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



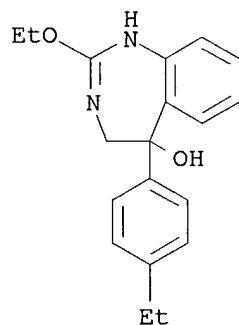
● HCl

RN 60330-71-4 CAPLUS
CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-4,5-dihydro-5-(4-methylphenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

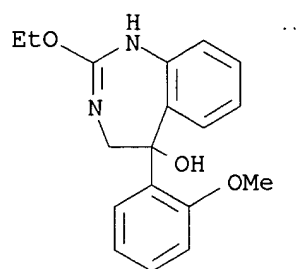
RN 60330-72-5 CAPLUS
CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-5-(4-ethylphenyl)-4,5-dihydro-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

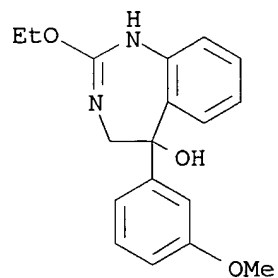
RN 60330-73-6 CAPLUS
CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-4,5-dihydro-5-(2-methoxyphenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)

10/019,683



● HCl

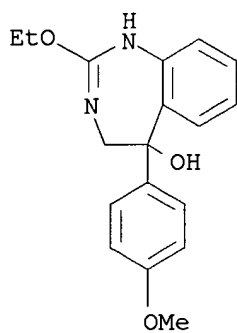
RN 60330-74-7 CAPLUS
CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-4,5-dihydro-5-(3-methoxyphenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 60330-75-8 CAPLUS
CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-4,5-dihydro-5-(4-methoxyphenyl)-,
monohydrochloride (9CI) (CA INDEX NAME)

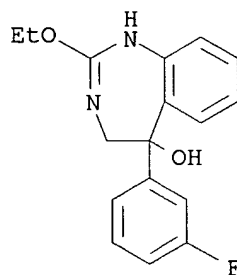
10/019,683



● HCl

RN 60330-76-9 CAPLUS

CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-5-(3-fluorophenyl)-4,5-dihydro-,
monohydrochloride (9CI) (CA INDEX NAME)

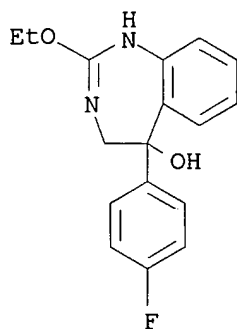


● HCl

RN 60330-77-0 CAPLUS

CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-5-(4-fluorophenyl)-4,5-dihydro-,
monohydrochloride (9CI) (CA INDEX NAME)

10/019,683

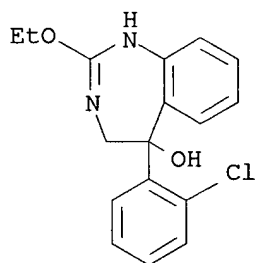


● HCl

RN 60330-79-2 CAPLUS
CN 1H-1,3-Benzodiazepin-5-ol, 5-(2-chlorophenyl)-2-ethoxy-4,5-dihydro-,
sulfate (1:1) (salt) (9CI) (CA INDEX NAME)

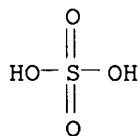
CM 1

CRN 60330-78-1
CMF C17 H17 Cl N2 O2



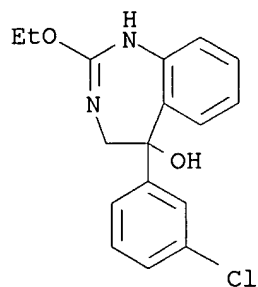
CM 2

CRN 7664-93-9
CMF H2 O4 S



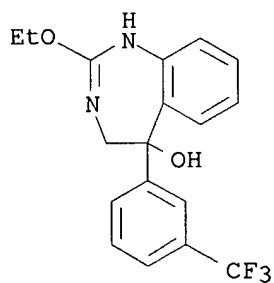
RN 60330-80-5 CAPLUS
CN 1H-1,3-Benzodiazepin-5-ol, 5-(3-chlorophenyl)-2-ethoxy-4,5-dihydro-,
monohydrochloride (9CI) (CA INDEX NAME)

10/019,683



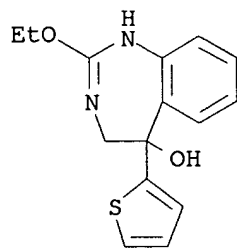
● HCl

RN 60330-81-6 CAPLUS
CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-4,5-dihydro-5-[3-(trifluoromethyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 60330-82-7 CAPLUS
CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-4,5-dihydro-5-(2-thienyl)-, monohydrochloride (9CI) (CA INDEX NAME)

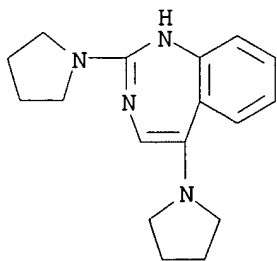


● HCl

10/019,683

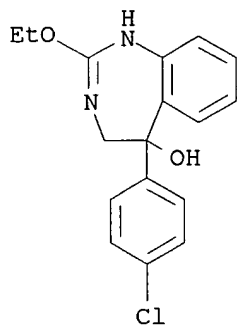
RN 60360-75-0 CAPLUS

CN 1H-1,3-Benzodiazepine, 2,5-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



RN 60407-42-3 CAPLUS

CN 1H-1,3-Benzodiazepin-5-ol, 5-(4-chlorophenyl)-2-ethoxy-4,5-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

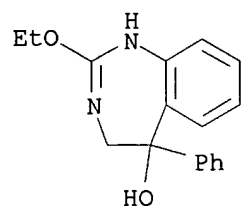
IT 60331-00-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, rearrangement, and decomposition of)

RN 60331-00-2 CAPLUS

CN 1H-1,3-Benzodiazepin-5-ol, 2-ethoxy-4,5-dihydro-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

10/019,683

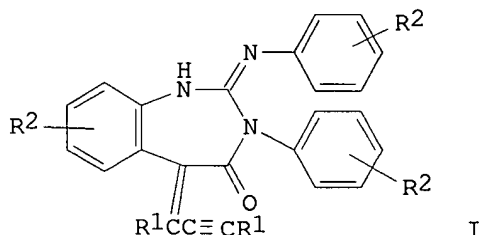


● HCl

10/019,683

10/019,683
X
L44 ANSWER 42 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:121912 CAPLUS
DOCUMENT NUMBER: 84:121912
TITLE: 1,3-Benzodiazepine derivatives
INVENTOR(S): Agawa, Toshio; Ohshiro, Yoshiki; Baba, Akio;
Matsumoto, Masaru
PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------------|------|----------|-----------------|------------|
| ----- | --- | ----- | ----- | ----- |
| JP 50121290 | A2 | 19750923 | JP 1974-28412 | 19740312 |
| PRIORITY APPLN. INFO.: GI | | | JP 1974-28412 | A 19740312 |

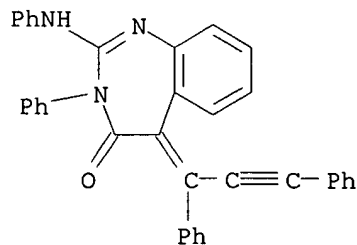


AB 1,3-Benzodiazepines I (R1 = aryl; R2 = H, alkyl) were prepared by reaction of acetylenes R1C.tplbond.CX (X = halo) with carbodiimides R2C6H4N:C:NC6H4R2 in the presence of Fe(CO)5. Thus, a mixture of Fe(CO)5 and PhN:C:NPh was heated, PhC.tplbond.CBr added, and the mixture stirred to give 40% I (R1 = Ph, R2 = H). I (R1 = Ph; R2 = 7-Me, 4'-Me, 4''-Me and R2 = 9-Me, 2'-Me, 2''-Me) were also prepared

IT 56185-26-3P 58678-50-5P 58678-51-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 56185-26-3 CAPLUS

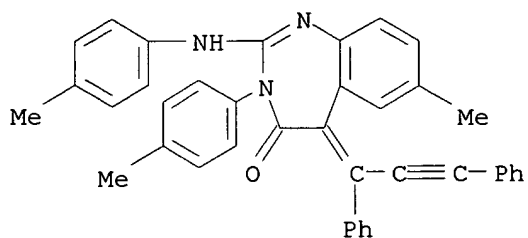
CN 4H-1,3-Benzodiazepin-4-one, 5-(1,3-diphenyl-2-propynylidene)-3,5-dihydro-3-phenyl-2-(phenylamino)- (9CI) (CA INDEX NAME)



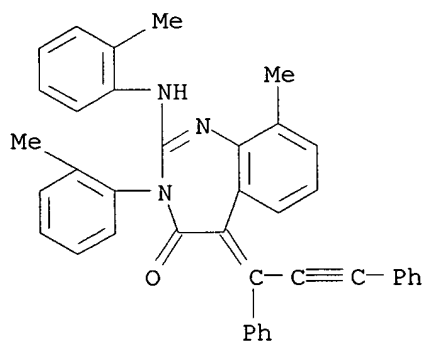
RN 58678-50-5 CAPLUS

10/019,683

CN 4H-1,3-Benzodiazepin-4-one, 5-(1,3-diphenyl-2-propynylidene)-1,2,3,5-tetrahydro-7-methyl-3-(4-methylphenyl)-2-[(4-methylphenyl)imino]- (9CI)
(CA INDEX NAME)



RN 58678-51-6 CAPLUS
CN 4H-1,3-Benzodiazepin-4-one, 5-(1,3-diphenyl-2-propynylidene)-1,2,3,5-tetrahydro-9-methyl-3-(2-methylphenyl)-2-[(2-methylphenyl)imino]- (9CI)
(CA INDEX NAME)



10/019,683

~~L14~~ ANSWER 43 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1976:59373 CAPLUS

DOCUMENT NUMBER: 84:59373

TITLE: 6,7-Dihydropyrimido[2,1-b][1,3]benzodiazepine

AUTHOR(S): Yale, Harry L.; Bennett, C. R.; Petigara, R. B.

CORPORATE SOURCE: Squibb Inst. Med. Res., Princeton, NJ, USA

SOURCE: Journal of Heterocyclic Chemistry (1975), 12(5), 1053-4

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

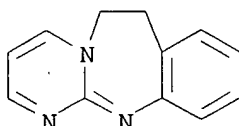
AB 2-Aminopyrimidine was treated with o-BrC₆H₄CH₂CH₂Br to give I, which was cyclized with copper bronze to give II.

IT 56119-83-6P 58061-91-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

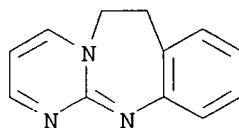
RN 56119-83-6 CAPLUS

CN Pyrimido[2,1-b][1,3]benzodiazepine, 6,7-dihydro- (9CI) (CA INDEX NAME)



RN 58061-91-9 CAPLUS

CN Pyrimido[2,1-b][1,3]benzodiazepine, 6,7-dihydro-, monohydrochloride (9CI)
(CA INDEX NAME)



● HCl

14 ANSWER 44 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1975:479208 CAPLUS

DOCUMENT NUMBER: 83:79208

TITLE: Reactions of phenylbromoacetylene with heterocumulenes in the presence of iron pentacarbonyl

AUTHOR(S): Baba, Akio; Ohshiro, Yoshiki; Agawa, Toshio

CORPORATE SOURCE: Fac. Eng., Osaka Univ., Suita, Japan

SOURCE: Journal of Organometallic Chemistry (1975), 87(2), 247-56

CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 83:79208

GI For diagram(s), see printed CA Issue.

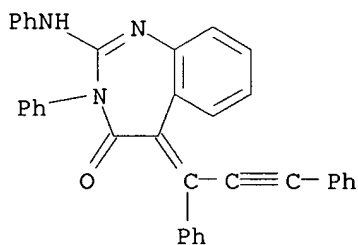
AB Reactions of PhC.tplbond.CBr7 with RN:C:NR1 in the presence of iron pentacarbonyl gave diazepinone derivs. I ($\text{R} = \text{Ph}$, $\text{R1} = \text{H}$; $\text{R} = \text{p-MeC}_6\text{H}_4$, $\text{R1} = 4\text{-Me}$; $\text{R} = \text{o-MeC}_6\text{H}_4$, $\text{R1} = 2\text{-Me}$) in 41-17% yields. The reaction with PhNCO gave two hydantoin derivs. II ($\text{R} = \text{H}$, PhC.tplbond.C) (8 and 18% resp.). The reaction with PhC:C:O was not catalyzed by iron pentacarbonyl and gave 2-bromo-3,4-diphenyl-1-diphenylacetoxynaphthalene. In all cases coupling of PhC.tplbond.CBr7 gave diphenylbutadiyne.

IT 56185-26-3P 56185-27-4P 56185-28-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

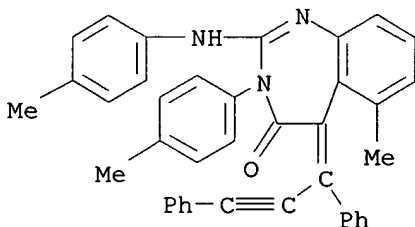
RN 56185-26-3 CAPLUS

CN 4H-1,3-Benzodiazepin-4-one, 5-(1,3-diphenyl-2-propynylydene)-3,5-dihydro-3-phenyl-2-(phenylamino)- (9CI) (CA INDEX NAME)



RN 56185-27-4 CAPLUS

CN 4H-1,3-Benzodiazepin-4-one, 5-(1,3-diphenyl-2-propynylydene)-3,5-dihydro-6-methyl-3-(4-methylphenyl)-2-[(4-methylphenyl)amino]- (9CI) (CA INDEX NAME)

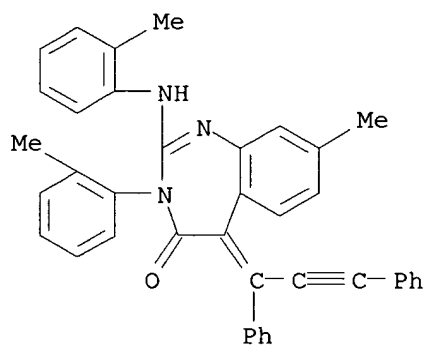


RN 56185-28-5 CAPLUS

CN 4H-1,3-Benzodiazepin-4-one, 5-(1,3-diphenyl-2-propynylydene)-3,5-dihydro-8-

10/019,683

methyl-3-(2-methylphenyl)-2-[(2-methylphenyl)amino]- (9CI) (CA INDEX
NAME)



10/019,683

104 ANSWER 45 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1975:458862 CAPLUS

DOCUMENT NUMBER: 83:58862

TITLE: Therapeutic compounds and intermediates

INVENTOR(S): Yale, Harry L.; Petigara, Ramesh B.

PATENT ASSIGNEE(S): E. R. Squibb and Sons, Inc., USA

SOURCE: U.S., 16 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| US 3868374 | A | 19750225 | US 1973-382804 | 19730726 |
| CA 1051885 | A1 | 19790403 | CA 1974-203632 | 19740628 |
| GB 1474252 | A | 19770518 | GB 1974-29534 | 19740703 |
| DE 2435384 | A1 | 19750213 | DE 1974-2435384 | 19740723 |
| FR 2238490 | A1 | 19750221 | FR 1974-26129 | 19740726 |
| FR 2238490 | B1 | 19780630 | | |
| JP 50041894 | A2 | 19750416 | JP 1974-86509 | 19740726 |
| US 3957787 | A | 19760518 | US 1974-532796 | 19741216 |
| US 4001233 | A | 19770104 | US 1976-651390 | 19760122 |
| PRIORITY APPLN. INFO.: | | | US 1973-382804 | A 19730726 |
| | | | US 1974-532796 | A3 19741216 |

GI For diagram(s), see printed CA Issue.

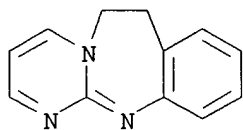
AB Pyrimidobenzodiazepine I (R = H, n = 2) and pyrimidobenzodiazocine I (R = MeS, n = 3), useful as central nervous system stimulants and muscle relaxants (no data), were prepared by cyclization of pyrimidinium bromide II. Thus, 2-BrC₆H₄CH₂OH underwent successively bromination, cyanation, hydrolysis, reduction with LiAlH₄, and bromination to give 2-BrC₆H₄CH₂Br which after condensation with 2-aminopyrimidine (III) gave II (R = H, n = 2) (IV). Cyclization by heating IV in presence of K₂CO₃ and copper bronze gave I (R = H, n = 2). Similarly cyclization of II (R = MeS, n = 3) (V) gave I (R = MeS, n = 3). The Grignard reaction of 2,5-Br(MeS)C₆H₃CH₂Br with ethylene oxide followed by bromination and condensation with III gave V.

IT 56119-83-6P 56119-84-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 56119-83-6 CAPLUS

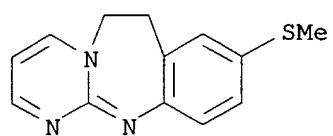
CN Pyrimido[2,1-b][1,3]benzodiazepine, 6,7-dihydro- (9CI) (CA INDEX NAME)



RN 56119-84-7 CAPLUS

CN Pyrimido[2,1-b][1,3]benzodiazepine, 6,7-dihydro-9-(methylthio)- (9CI) (CA INDEX NAME)

10/019,683



L14 ANSWER 46 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1975:73041 CAPLUS
 DOCUMENT NUMBER: 82:73041
 TITLE: 2-(Substituted anilino)-4,5-dihydro-3H-1,3-benzodiazepines
 INVENTOR(S): Suh, John T.; Schnettler, Richard A.
 SOURCE: U.S., 3 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|------------|
| US 3849400 | A | 19741119 | US 1972-268127 | 19720630 |
| PRIORITY APPLN. INFO.: | | | US 1972-268127 | A 19720630 |

GI For diagram(s), see printed CA Issue.

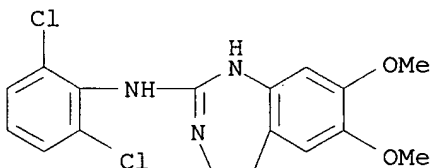
AB Benzodiazepines I (R = H, OMe; R1 = 2,6-Cl₂C₆H₃, 2-CF₃C₆H₄, 4-ClC₆H₄) were prepared by treating the aminophenethylamines II with RN:CCl₂. I were central nervous depressants in mice at 10 mg/kg i.p. and lowered the blood pressure in cats at 10 mg/kg i.v.

IT 55474-29-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and pharmacol. activity)

RN 55474-29-8 CAPLUS

CN 3H-1,3-Benzodiazepin-2-amine, N-(2,6-dichlorophenyl)-4,5-dihydro-7,8-dimethoxy- (9CI) (CA INDEX NAME)

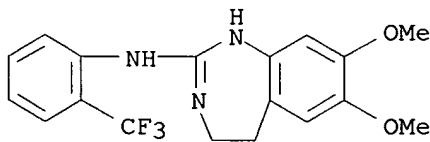


IT 55474-32-3P 55474-33-4P 55474-34-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and pharmacol. activity of)

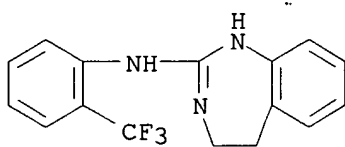
RN 55474-32-3 CAPLUS

CN 3H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-7,8-dimethoxy-N-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



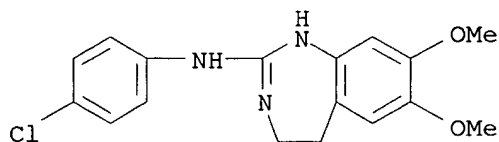
RN 55474-33-4 CAPLUS

CN 3H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 55474-34-5 CAPLUS

CN 3H-1,3-Benzodiazepin-2-amine, N-(4-chlorophenyl)-4,5-dihydro-7,8-dimethoxy- (9CI) (CA INDEX NAME)

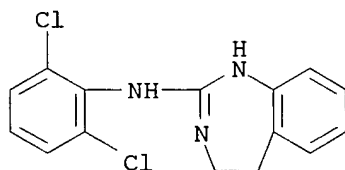


IT 55474-30-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 55474-30-1 CAPLUS

CN 3H-1,3-Benzodiazepin-2-amine, N-(2,6-dichlorophenyl)-4,5-dihydro- (9CI)
(CA INDEX NAME)



L14 ANSWER 47 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1975:4327 CAPLUS

DOCUMENT NUMBER: 82:4327

TITLE: 2-Heterocyclic-1,3-benzodiazepines

INVENTOR(S): Suh, John T.; Schnettler, Richard A.

SOURCE: U.S., 3 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|------------|
| ----- | ---- | ----- | ----- | ----- |
| US 3838122 | A | 19740924 | US 1972-268128 | 19720630 |
| PRIORITY APPLN. INFO.: | | | US 1972-268128 | A 19720630 |

GI For diagram(s), see printed CA Issue.

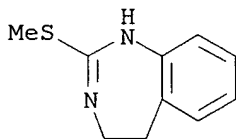
AB The benzodiazepines I (R = MeS, morpholino, 4-methyl-1-piperazinyl 1-pyrrolidinyl, etc.; R1 = H, MeO) were prepared Thus, 2,4,5-O2N(MeO)2C6H2CH2CH2NH2 was hydrogenated and treated with CS2 to give 7,8-dimethoxy-2,3,4,5-tetrahydro-1H-1,3-benzodiazepine-2-thione, which was methylated with MeI and the resulting I (R = MeS, R1 = MeO). HI treated with morpholine to give I (R = morpholino, R1 = MeO). At 30-300 mg/kg I were muscle relaxants and at 10 mg/kg were antihypertensives.

IT 54047-05-1P 54047-07-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with amines)

RN 54047-05-1 CAPLUS

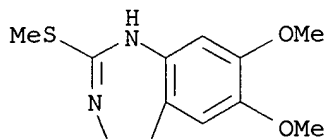
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(methylthio)-, hydriodide (9CI) (CA INDEX NAME)



●x HI

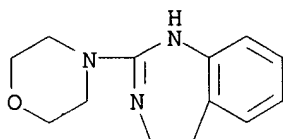
RN 54047-07-3 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-7,8-dimethoxy-2-(methylthio)-, hydriodide (9CI) (CA INDEX NAME)



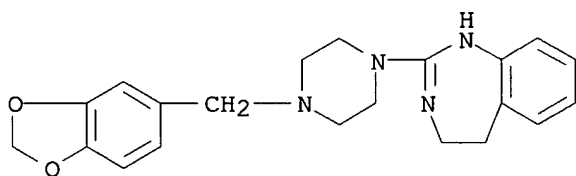
●x HI

IT 54047-01-7P 54047-02-8P 54047-03-9P
 54047-04-0P 54047-06-2P 54047-08-4P
 54047-09-5P 54047-10-8P 54047-11-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 54047-01-7 CAPLUS
 CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(4-morpholinyl)-, hydriodide (9CI)
 (CA INDEX NAME)



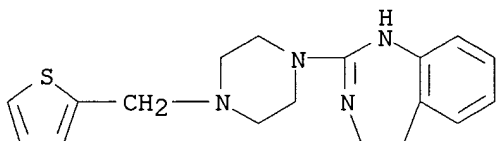
●x HI

RN 54047-02-8 CAPLUS
 CN 1H-1,3-Benzodiazepine, 2-[4-(1,3-benzodioxol-5-ylmethyl)-1-piperazinyl]-
 4,5-dihydro-, hydriodide (9CI) (CA INDEX NAME)



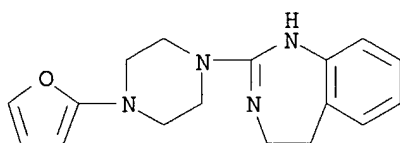
●x HI

RN 54047-03-9 CAPLUS
 CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-[4-(2-thienylmethyl)-1-piperazinyl]-,
 hydriodide (9CI) (CA INDEX NAME)



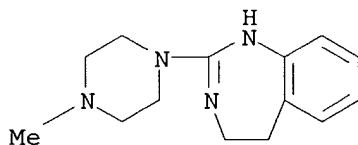
●x HI

RN 54047-04-0 CAPLUS
CN 1H-1,3-Benzodiazepine, 2-[4-(2-furanyl)-1-piperazinyl]-4,5-dihydro-, hydriodide (9CI) (CA INDEX NAME)



●x HI

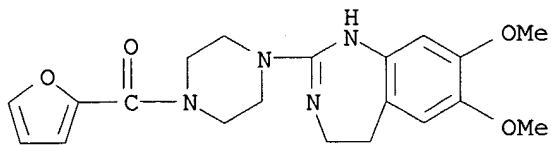
RN 54047-06-2 CAPLUS
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(4-methyl-1-piperazinyl)-, hydriodide (9CI) (CA INDEX NAME)



●x HI

RN 54047-08-4 CAPLUS
CN Piperazine, 1-(4,5-dihydro-7,8-dimethoxy-1H-1,3-benzodiazepin-2-yl)-4-(2-furanylcarbonyl)-, hydriodide (9CI) (CA INDEX NAME)

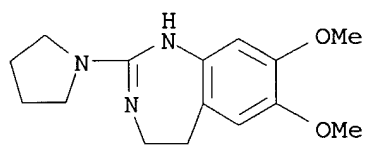
10/019,683



●x HI

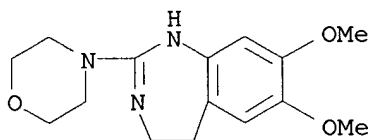
RN 54047-09-5 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-7,8-dimethoxy-2-(1-pyrrolidinyl)- (9CI)
(CA INDEX NAME)



RN 54047-10-8 CAPLUS

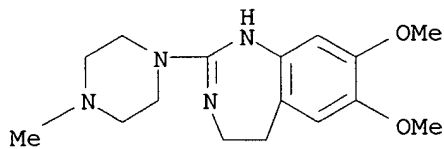
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-7,8-dimethoxy-2-(4-morpholinyl)-,
hydriodide (9CI) (CA INDEX NAME)



●x HI

RN 54047-11-9 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-7,8-dimethoxy-2-(4-methyl-1-
piperazinyl)-, hydriodide (9CI) (CA INDEX NAME)



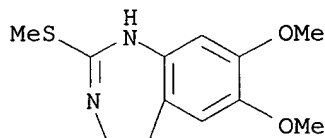
●x HI

L14 ANSWER 48 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1974:83080 CAPLUS
 DOCUMENT NUMBER: 80:83080
 TITLE: 2-(Aralkylamino)-4,5-dihydro-3H-1,3-benzodiazepines
 INVENTOR(S): Suh, John T.; Schnettler, Richard A.
 SOURCE: U.S., 3 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

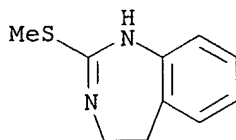
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|------------|
| US 3780023 | A | 19731218 | US 1972-268129 | 19720630 |
| PRIORITY APPLN. INFO.: | | | US 1972-268129 | A 19720630 |

GI For diagram(s), see printed CA Issue.
 AB The benzodiazepines I (R = PhCH₂CH₂NH, PhCH₂NH, 3,4-(MeO)₂C₆H₃CH₂CH₂NH) were prepared Thus, o-H₂NC₆H₄CH₂CH₂NH₂ was treated with CS₂ and the resulting 2,3,4,5-tetrahydro-1H-1,3-benzodiazepine-2-thione methylated with MeI to give I (R = MeS).HI, which with PhCH₂CH₂NH₂ gave I (R = PhCH₂CH₂NH).HI. At 1-10 mg/kg I (R = PhCH₂NH) was a tranquilizer. The LD₅₀ of I were 20 mg/kg.
 IT 37852-20-3P 52063-46-4P 52063-51-1P
 52063-52-2P 52063-53-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 37852-20-3 CAPLUS
 CN 1H-1,3-Benzodiazepine, 4,5-dihydro-7,8-dimethoxy-2-(methylthio)-, monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 52063-46-4 CAPLUS
 CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(methylthio)-, monohydriodide (9CI)
 (CA INDEX NAME)

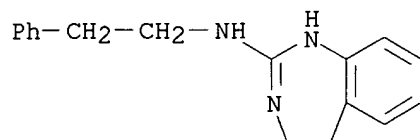


● HI

10/019,683

RN 52063-51-1 CAPLUS

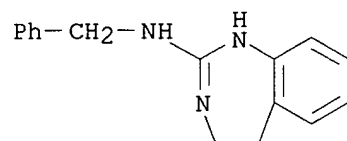
CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-(2-phenylethyl)-,
monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 52063-52-2 CAPLUS

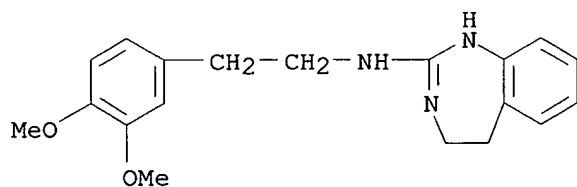
CN 1H-1,3-Benzodiazepin-2-amine, 4,5-dihydro-N-(phenylmethyl)-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52063-53-3 CAPLUS

CN 1H-1,3-Benzodiazepin-2-amine, N-[2-(3,4-dimethoxyphenyl)ethyl]-4,5-dihydro-
, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L14 ANSWER 49 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1974:83079 CAPLUS
 DOCUMENT NUMBER: 80:83079
 TITLE: 2-(Aminoalkylamino)-4,5-dihydro-3h-1,3-benzodiazepines
 INVENTOR(S): Suh, John T.; Schnettler, Richard A.
 SOURCE: U.S., 3 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|------------|
| US 3780024 | A | 19731218 | US 1972-268130 | 19720630 |
| PRIORITY APPLN. INFO.: | | | US 1972-268130 | A 19720630 |

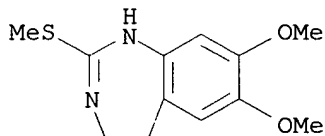
GI For diagram(s), see printed CA Issue.

AB The benzodiazepines I [R = Me₂N(CH₂)₃NH, Me₂NCH₂CH₂NH, R₁ = H, MeO] were prepared. Thus, 2,4,5-(OMe)₃2C₆H₂CH₂CH₂NH₂ was hydrogenated over PtO and the product treated with CS₂ to give 7,8-dimethoxy-2,3,4,5-tetrahydro-1H-1,3-benzodiazepine-2-thione, which was methylated with MeI and the resulting I (R = SMe, R₁ = MeO). HI treated with Me₂N(CH₂)₃NH₂ to give I (R = Me₂N(CH₂)₃NH, R₁ = MeO). At 30-300 mg/kg I (R = Me₂NCH₂CH₂NH, R₁ = H) (II) caused central nervous system depression. The LD₅₀ of II was >75 mg/kg. At 10 mg/kg II reduced blood pressure in cats.

IT 37852-20-3P 52063-46-4P 52063-47-5P
 52063-48-6P 52063-49-7P 52063-50-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 37852-20-3 CAPLUS

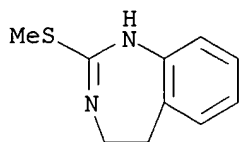
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-7,8-dimethoxy-2-(methylthio)-,
 monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 52063-46-4 CAPLUS

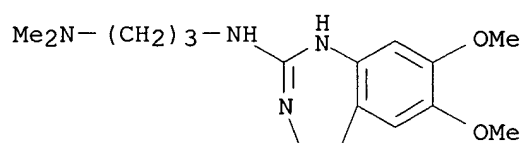
CN 1H-1,3-Benzodiazepine, 4,5-dihydro-2-(methylthio)-, monohydriodide (9CI)
 (CA INDEX NAME)



● HI

RN 52063-47-5 CAPLUS

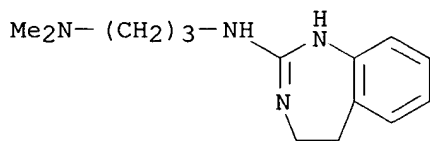
CN 1,3-Propanediamine, N'-(4,5-dihydro-7,8-dimethoxy-1H-1,3-benzodiazepin-2-yl)-N,N-dimethyl-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

RN 52063-48-6 CAPLUS

CN 1,3-Propanediamine, N'-(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)-N,N-dimethyl-, dihydrochloride (9CI) (CA INDEX NAME)

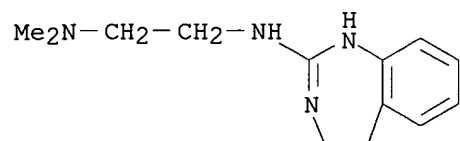


● 2 HCl

RN 52063-49-7 CAPLUS

CN 1,2-Ethanediamine, N'-(4,5-dihydro-1H-1,3-benzodiazepin-2-yl)-N,N-dimethyl-, dihydrochloride (9CI) (CA INDEX NAME)

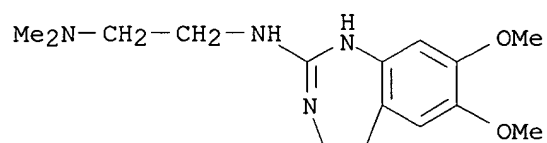
10/019,683



● 2 HCl

RN 52063-50-0 CAPLUS

CN 1,2-Ethanediamine, N'-(4,5-dihydro-7,8-dimethoxy-1H-1,3-benzodiazepin-2-yl)-N,N-dimethyl-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

10/019,683

~~L14~~ ANSWER 50 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1973:449091 CAPLUS

DOCUMENT NUMBER: 79:49091

TITLE: Amidines. 4. Synthesis of tricyclic guanidines related to 1,2,3,5-tetrahydroimidazo[2,1-b]quinazoline, a new antihypertensive agent

AUTHOR(S): Jen, Timothy; Bender, Paul; Van Hoeven, Helen; Dienel, Barbara; Loev, Bernard

CORPORATE SOURCE: Res. Dev. Div., Smith Kline and French Lab., Philadelphia, PA, USA

SOURCE: Journal of Medicinal Chemistry (1973), 16(4), 407-11
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 1,2,3,5-Tetrahydroimidazo[2,1-b]quinazoline-HCl (I-HCl) [33376-05-5], 1,2,3,4-tetrahydro-6H-pyrimido[2,1-b]quinazoline-HBr (II-HBr) [41363-26-2], and 2,3-dihydro-1H-imidazo[1,2-a]benzimidazole-HCl (III-HCl) [41363-27-3] showed antihypertensive activity at 2.5, 2, and 10 mg/kg orally, resp., in neurogenic hypertensive dogs. In metacorticoid hypertensive rats, II was less potent than I in lowering systolic pressure.

IT 41921-54-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and antihypertensive activity of)

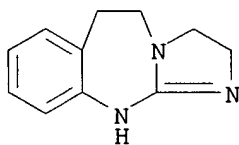
RN 41921-54-4 CAPLUS

CN 1H-Imidazo[2,1-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro-, compd. with 2,4,6-trinitrophenol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 41921-69-1

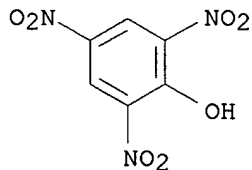
CMF C11 H13 N3



CM 2

CRN 88-89-1

CMF C6 H3 N3 O7



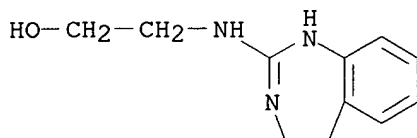
10/019,683

IT 41921-64-6P 41921-69-1P 41968-09-6P
42075-58-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 41921-64-6 CAPLUS

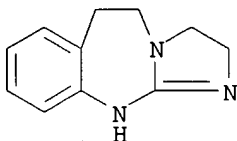
CN Ethanol, 2-[(4,5-dihydro-3H-1,3-benzodiazepin-2-yl)amino]-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

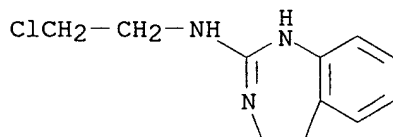
RN 41921-69-1 CAPLUS

CN 1H-Imidazo[2,1-b][1,3]benzodiazepine, 2,3,5,6-tetrahydro- (9CI) (CA INDEX NAME)



RN 41968-09-6 CAPLUS

CN 3H-1,3-Benzodiazepin-2-amine, N-(2-chloroethyl)-4,5-dihydro-,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 42075-58-1 CAPLUS

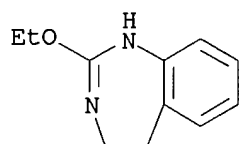
CN 3H-1,3-Benzodiazepine, 2-ethoxy-4,5-dihydro-, mono[tetrafluoroborate(1-)]-
(9CI) (CA INDEX NAME)

CM 1

CRN 48142-00-3

CMF C11 H14 N2 O

10/019,683

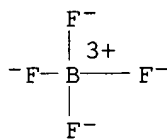


CM 2

CRN 16872-11-0

CMF B F4 . H

CCI CCS



L14 ANSWER 51 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1972:540178 CAPLUS
 DOCUMENT NUMBER: 77:140178
 TITLE: Pharmacologically active 1,3-benzodiazepines
 INVENTOR(S): Rodriguez, Herman Robert; De Stevens, George
 SOURCE: U.S., 12 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| US 3681340 | A | 19720801 | US 1968-704517 | 19680212 |
| US 3862228 | A | 19750121 | US 1972-227619 | 19720218 |
| PRIORITY APPLN. INFO.: | | | US 1967-630520 | A2 19670413 |
| | | | US 1967-649828 | A2 19670629 |
| | | | US 1968-704517 | A2 19680212 |
| | | | US 1970-10649 | A2 19700211 |

GI For diagram(s), see printed CA Issue.

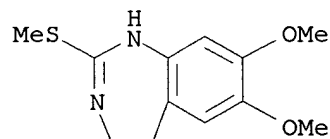
AB The diazepines (I, R = H, MeO, iso-BuO, R1 = e.g., HO, H2N, MeS, HS, MeOCH2, Ph, PhCH2, p-F3-CC6H4, m- or p-ClC6H4, m- or p-FC6H4, R2 = H, Me) and their acid salts, useful as analgesics, tranquilizers, and agents to increase coronary blood flow, are prepared by cyclizing amidines (II, R3 = O2N, H2N). Thus, II (R = MeO, R1 = Ph, R2 = H, R3 = H2N) was refluxed in toluene and treated with HCl-EtOH to give I-HCl. The II are prepared by treating the imidic acids R1C-(:NH)OH with 2,4,5-O2N(MeO)2C6H2CH2CH2NH2-HCl to give the II (R3 = O2N) which are hydrogenated to II (R3 = H2N).

IT 37852-20-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 37852-20-3 CAPLUS

CN 1H-1,3-Benzodiazepine, 4,5-dihydro-7,8-dimethoxy-2-(methylthio)-,
 monohydriodide (9CI) (CA INDEX NAME)



● HI

10/019,683

~~124~~ ANSWER 52 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1969:524388 CAPLUS

DOCUMENT NUMBER: 71:124388

TITLE: Substituted 1,3-dihydro-4H-furo[3,4-d]-1,3-benzodiazepin-3-ones: synthesis and scope of the method

AUTHOR(S): Venturella, Vincent S.; Watson, Edward John, Jr.

CORPORATE SOURCE: Sch. of Pharm., Temple Univ., Nutley, NJ, USA

SOURCE: Journal of Heterocyclic Chemistry (1969), 6(5), 671-9

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 71:124388

GI For diagram(s), see printed CA Issue.

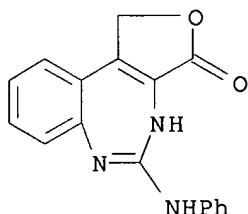
AB The preparation of a series of 1,3-dihydro-4H-furo-[3,4-d]-1,3-benzodiazepin-3-ones (I) was studied. This study and the I prepared tend to illustrate that the limiting factor in the scope of the synthetic method is similar to that noted generally in the Fischer indole synthesis. The lactone ring is relatively stable under a variety of conditions, and is believed to lend ease of formation to the ring system studied.

IT 24188-33-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 24188-33-8 CAPLUS

CN 3H-Furo[3,4-d][1,3]benzodiazepin-3-one, 5-anilino-1,4-dihydro-,
monohydrochloride (8CI) (CA INDEX NAME)



● HCl

10/019,683

114 ANSWER 53 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1969:491441 CAPLUS

DOCUMENT NUMBER: 71:91441

TITLE: 5,6-Dihydro-6-methylthiazolo-[2,3-b] [1,3] benzodiazepines, 2,3,10, 11-tetrahydro-10-methyl-1H-cyclopenta [4,5]thiazolo[2,3-b][1,3] benzodiazepine, and 7,8,9,10,12,13-hexahydro-13-methylbenzothiazolo[2,3-b][1,3]-benzodiazepine via 1,3,4,5-tetrahydro-5-methyl-2H-1,3-benzodiazepine-2-thione

AUTHOR(S): Elslager, Edward F.; Worth, Donald, F.

CORPORATE SOURCE: Med. and Sci. Affairs Div., Parke, Davis and Co., Ann Arbor, MI, USA

SOURCE: Journal of Heterocyclic Chemistry (1969), 6(4), 491-5
CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 71:91441

GI For diagram(s), see printed CA Issue.

AB Catalytic reductive scission of 4-methylcinnoline with Raney Ni afforded 57% o-amino-β-methylphenethylamine, treatment of which with CS₂ followed by thermal cyclization of the product furnished 1,3,4,5-tetrahydro-5-methyl-2H-1,3-benzodiazepine-2-thione (I). Reaction of I with ethyl chloroacetate, ethyl 2-bromohexanoate, ethyl 2-chloroacetoacetate, 2-bromo-2'-methoxyacetophenone, and 2-bromoacetophenone provided a series of substituted 5,6-dihydro-6-methylthiazolo[2,3-b][1,3]benzodiazepines. Condensation of I with 2-chlorocyclopentanone and 2-chlorocyclohexanone gave 2,3,10,11-tetrahydro-10-methyl-1H-cyclopenta[4,5]thiazolo-[2,3-b][1,3]benzodiazepine and 7,8,9,10,12,13-hexahydro-13-methylbenzothiazolo[2,3-b][1,3]benzodiazepine, resp. Structure assignments are discussed. None of the compds. possessed appreciable biol. activity.

IT 23890-69-9P 23890-70-2P 23890-71-3P

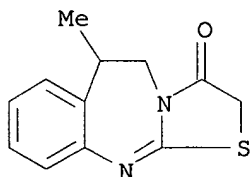
23890-72-4P 23890-73-5P 23890-74-6P

23890-75-7P 23921-51-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

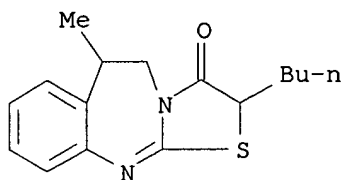
RN 23890-69-9 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepin-3(2H)-one, 5,6-dihydro-6-methyl- (8CI)
(CA INDEX NAME)



RN 23890-70-2 CAPLUS

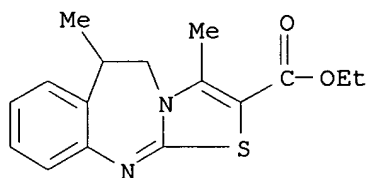
CN Thiazolo[2,3-b][1,3]benzodiazepin-3(2H)-one, 2-butyl-5,6-dihydro-6-methyl-, monohydrochloride (8CI) (CA INDEX NAME)



● HCl

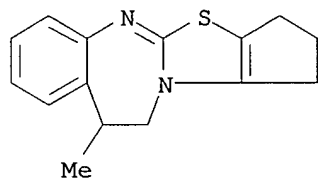
RN 23890-71-3 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine-2-carboxylic acid, 5,6-dihydro-3,6-dimethyl-, ethyl ester (8CI) (CA INDEX NAME)



RN 23890-72-4 CAPLUS

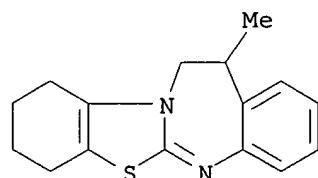
CN 1H-Cyclopenta[4,5]thiazolo[2,3-b][1,3]benzodiazepine, 2,3,10,11-tetrahydro-10-methyl-, hydrochloride (8CI) (CA INDEX NAME)



●x HCl

RN 23890-73-5 CAPLUS

CN Benzothiazolo[2,3-b][1,3]benzodiazepine, 7,8,9,10,12,13-hexahydro-13-methyl- (8CI) (CA INDEX NAME)

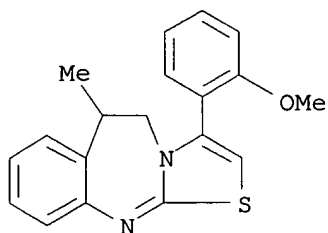


RN 23890-74-6 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-3-(o-methoxyphenyl)-6-

10/019,683

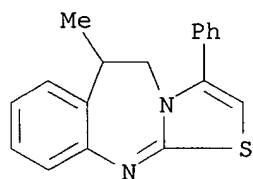
methyl-, monohydrobromide (8CI) (CA INDEX NAME)



● HBr

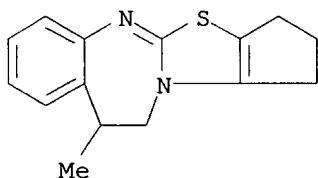
RN 23890-75-7 CAPLUS

CN Thiazolo[2,3-b][1,3]benzodiazepine, 5,6-dihydro-6-methyl-3-phenyl- (8CI)
(CA INDEX NAME)



RN 23921-51-9 CAPLUS

CN 1H-Cyclopenta[4,5]thiazolo[2,3-b][1,3]benzodiazepine, 2,3,10,11-tetrahydro-10-methyl- (8CI) (CA INDEX NAME)



114 ANSWER 54 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1965:91047 CAPLUS
 DOCUMENT NUMBER: 62:91047
 ORIGINAL REFERENCE NO.: 62:16281e-h,16282a-b
 TITLE: 6-Amino-5H-dibenzo[d,f] [1,3]diazepines
 INVENTOR(S): Kreighbaum, William E.; Scarborough, Homer C.
 PATENT ASSIGNEE(S): Mead Johnson & Co.
 SOURCE: 8 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|----------|
| US 3177202 | | 19650406 | US 1963-316140 | 19631014 |
| GB 1021941 | | | GB | |
| PRIORITY APPLN. INFO.: | | | US | 19631014 |

OTHER SOURCE(S): MARPAT 62:91047

GI For diagram(s), see printed CA Issue.

AB The title compds. are prepared by treating (a) I (R = SMe) with an amine, (b) 2,2'-diaminobiphenyl (II) with a dialkylcarbodiimide, or (c) II with an alkylisothiourea. Thus, a solution of 31.5 g. I, (R = SH) (Le Fevre, CA 23, 3456) in 260 ml. tetrahydrofuran is stirred with 21 g. MeI 2 hrs., the mixture allowed to stand overnight, the solid collected and air dried to give 41 g. I (R = SMe, HI salt) (III), m. 233-5° (decomposition). Treating a CHCl₃ solution of III with 5% aqueous KOH yields the free base (IV), m. 165-6°. Treating a tetrahydrofuran solution of IV with dry HCl in EtOH affords the HCl salt (V), m. 223-4° (decomposition). A mixture of 3 g. IV and 2 g. N,N-diethyl-N'-methylethylenediamine is heated to 200° 3 hrs., the mixture cooled, mixed with 30 ml. H₂O, the liquid decanted, the gum washed with 50 ml. MeOH, the solvent removed by distillation, the product converted to the dihydrochloride by treatment with 5N HCl in EtOH, and twice recrystd. from EtOH-iso-Pr₂O to give 81% I, R = NMe(CH₂)₂NEt₂, m. 249-50° (decomposition). Similarly is obtained from III 87% I (R = piperidino), m. 142-3°; and from V the dihydrochloride of I [R = (2-morpholinoethyl)amino], m. 279-80° (decomposition). A mixture of 9.2 g. II and 6.5 g.

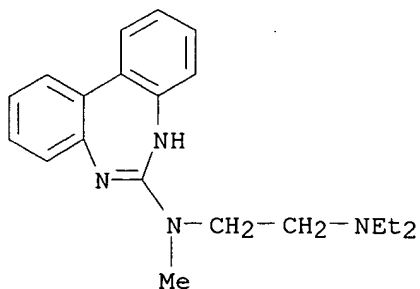
N,N'-diisopropylcarbodiimide

is heated to 150° (the reaction proceeds briskly at 170° with a strong amine evolution), the temperature held at 190-200° 0.5 hr., the melt allowed to cool, and recrystd. once from EtOH-EtOAc and once from iso-PrOH to give 80% I (R = NHPr-iso), m. 222.0-2.5°. Similarly are obtained 6-isopropylamino-3,9-dimethyl-5H-dibenzo[d,f][1,3]diazepine, m. 239-40°; I (R = cyclohexylamino), m. 231-2°. A mixture of 6 g. II and 6 g. S-methylpseudothiouthiourea sulfate is heated to 100°, the temperature gradually raised to 200°, and held there 0.5 hr., the gum cooled, collected, triturated with 200 ml. H₂O and the insol. solid recrystd. from 35% EtOH to yield 36% I (R = NH₂), m. 208-9° (decomposition). Similarly are obtained the following I (R, salt, m.p., given): hexamethylenimino, ethanol complex, 69-80° (decomposition); 4-methylpiperazino, di-HCl, >310°; NMe(CH₂)₂NMe₂, di-HCl, 250-1°; NEt(CH₂)₂NEt₂, di-HCl, 159-61°; NMe₂, HCl, >310°; NEt₂, HCl, >310°; NHMe, --, 243-5°; NHET, --, 213-15°; morpholino, HCl, >310°; pyrrolidino, HCl, >310°; 2-thiazolylamino, --, 204-5°; NHBu, HCl, 239-41°; anilino, --, 255-6°; NH(CH₂)₂NMe₂, di-HCl, 219-21°; 6-(2-morpholinoethylamino)-3,9-dichloro-5H-

dibenzo[d,f][1,3]diazepine, --, 215.5-17.5°; carbethoxymethylamino, HCl, 193-4° (decomposition); NHOH, HCl, 225-6° (decomposition). (uv and ir data are tabulated). The compds. and the salts thereof with pharmaceutically acceptable acids possess antifungal, antibacterial, anticonvulsant, muscle relaxant, interneuronal depressant, and a variety of psychotropic effects.

- IT 2849-00-5, 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(diethylamino)ethyl]methylamino]-, dihydrochloride 2849-01-6, 5H-Dibenzo[d,f][1,3]diazepine, 6-piperidino- 2849-02-7, 5H-Dibenzo[d,f][1,3]diazepine, 6-(isopropylamino)-3,9-dimethyl- 2849-04-9, 5H-Dibenzo[d,f][1,3]diazepine, 6-(dimethylamino)-, hydrochloride 2849-05-0, 5H-Dibenzo[d,f][1,3]diazepine, 6-(methylamino)- 2849-06-1, 5H-Dibenzo[d,f][1,3]diazepine, 6-(ethylamino)- 2849-07-2, 5H-Dibenzo[d,f][1,3]diazepine, 6-morpholino-, hydrochloride 2849-08-3, 5H-Dibenzo[d,f][1,3]diazepine, 6-(1-pyrrolidinyl)-, hydrochloride 2849-09-4, 5H-Dibenzo[d,f][1,3]diazepine, 6-(2-thiazolylamino)- 2849-31-2, 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(diethylamino)ethyl]amino]-, dihydrochloride 2849-32-3, 5H-Dibenzo[d,f][1,3]diazepine, 6-(butylamino)-, hydrochloride 2849-34-5, 5H-Dibenzo[d,f][1,3]diazepine, 3,9-dichloro-6-[[2-morpholinoethyl]amino]- 2849-35-6, 5H-Dibenzo[d,f][1,3]diazepine, 6-(hydroxyamino)-, hydrochloride 2870-28-2, 5H-Dibenzo[d,f][1,3]diazepine, 6-(hexahydro-1H-azepin-1-yl)-, compound with EtOH (1:1) 2880-29-7, 5H-Dibenzo[d,f][1,3]diazepine, 6-(methylthio)- 2880-30-0, 5H-Dibenzo[d,f][1,3]diazepine, 6-(isopropylamino)- 2880-31-1, 5H-Dibenzo[d,f][1,3]diazepine, 6-(cyclohexylamino)- 2880-32-2, 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(dimethylamino)ethyl]methylamino]-, dihydrochloride 2880-33-3, 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(diethylamino)ethyl]ethylamino]-, dihydrochloride 2880-34-4, 5H-Dibenzo[d,f][1,3]diazepine, 6-(diethylamino)-, hydrochloride 2880-35-5, 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(dimethylamino)ethyl]amino]-, dihydrochloride 2880-36-6, Glycine, N-5H-dibenzo[d,f][1,3]diazepin-6-yl-, ethyl ester, hydrochloride 2882-40-8, 5H-Dibenzo[d,f][1,3]diazepine, 6-(methylthio)-, hydriodide 3048-94-0, 5H-Dibenzo[d,f][1,3]diazepine, 6-(hexahydro-1H-azepin-1-yl)- 3048-97-3, 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-morpholinoethyl]amino]-, dihydrochloride 3048-98-4, 5H-Dibenzo[d,f][1,3]diazepine, 6-(4-methyl-1-piperazinyl)-, dihydrochloride (preparation of)
- RN 2849-00-5 CAPLUS
- CN 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(diethylamino)ethyl]methylamino]-, dihydrochloride (7CI, 8CI) (CA INDEX NAME)

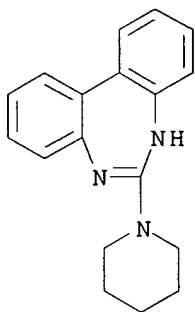
10/019,683



● 2 HCl

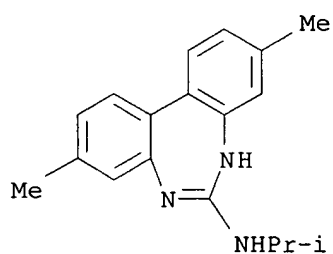
RN 2849-01-6 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(1-piperidiny)- (9CI) (CA INDEX NAME)



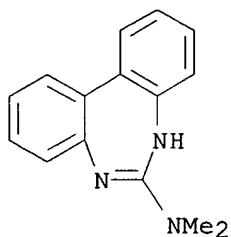
RN 2849-02-7 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(isopropylamino)-3,9-dimethyl- (7CI, 8CI)
(CA INDEX NAME)



RN 2849-04-9 CAPLUS

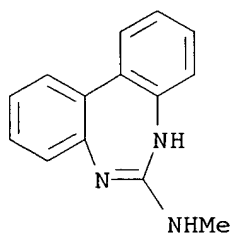
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(dimethylamino)-, monohydrochloride (8CI)
(CA INDEX NAME)



● HCl

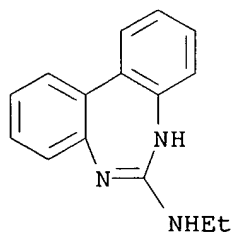
RN 2849-05-0 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepin-6-amine, N-methyl- (9CI) (CA INDEX NAME)



RN 2849-06-1 CAPLUS

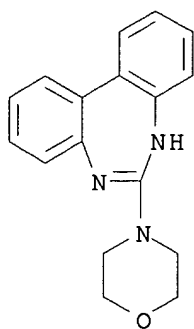
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(ethylamino)- (7CI, 8CI) (CA INDEX NAME)



RN 2849-07-2 CAPLUS

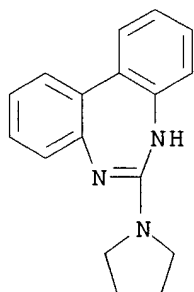
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-morpholino-, monohydrochloride (8CI) (CA INDEX NAME)

10/019,683



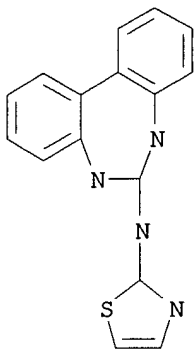
● HCl

RN 2849-08-3 CAPLUS
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(1-pyrrolidinyl)-, monohydrochloride
(8CI) (CA INDEX NAME)



● HCl

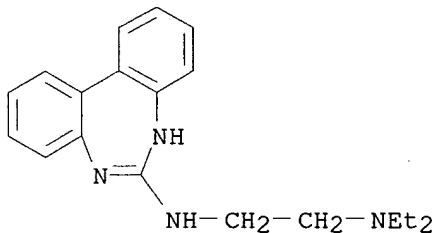
RN 2849-09-4 CAPLUS
CN 5H-Dibenzo[d,f][1,3]diazepin-6-amine, N-(2-thiazolyl)- (9CI) (CA INDEX
NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 2849-31-2 CAPLUS

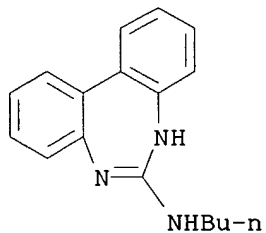
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-[[[(diethylamino)ethyl]amino]-, dihydrochloride (8CI) (CA INDEX NAME)



● 2 HCl

RN 2849-32-3 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(butylamino)-, monohydrochloride (8CI) (CA INDEX NAME)

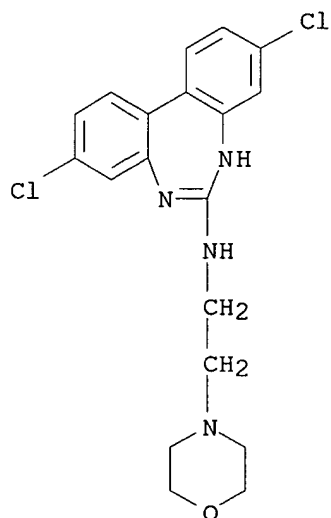


● HCl

RN 2849-34-5 CAPLUS

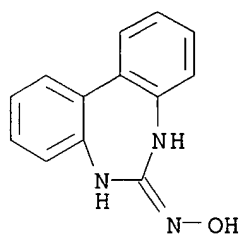
CN 5H-Dibenzo[d,f][1,3]diazepine, 3,9-dichloro-6-[(2-morpholinoethyl)amino]-, dihydrochloride (7CI, 8CI) (CA INDEX NAME)

10/019,683



RN 2849-35-6 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(hydroxyamino)-, monohydrochloride (8CI)
(CA INDEX NAME)



● HCl

RN 2870-28-2 CAPLUS

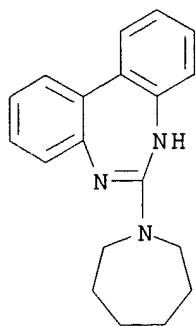
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(hexahydro-1H-azepin-1-yl)-, compd. with
ethanol (1:1) (8CI) (CA INDEX NAME)

CM 1

CRN 3048-94-0

CMF C19 H21 N3

10/019,683



CM 2

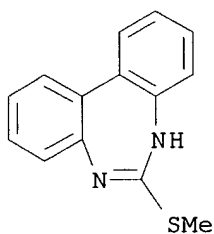
CRN 64-17-5

CMF C2 H6 O

H₃C-CH₂-OH

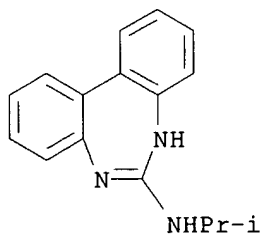
RN 2880-29-7 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(methylthio)- (7CI, 8CI, 9CI) (CA INDEX NAME)



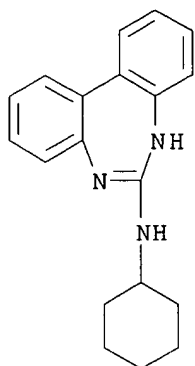
RN 2880-30-0 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(isopropylamino)- (7CI, 8CI) (CA INDEX NAME)

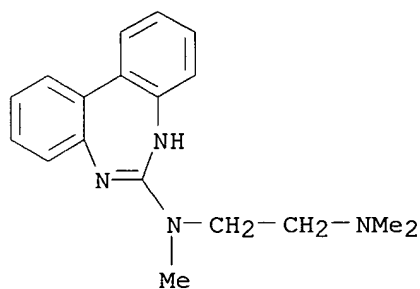


RN 2880-31-1 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(cyclohexylamino)- (7CI, 8CI) (CA INDEX NAME)

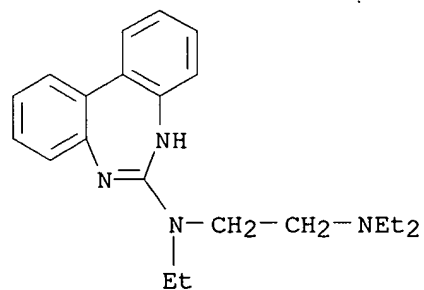


RN 2880-32-2 CAPLUS
 CN 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(dimethylamino)ethyl]methylamino]-, dihydrochloride (7CI, 8CI) (CA INDEX NAME)



● 2 HCl

RN 2880-33-3 CAPLUS
 CN 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(diethylamino)ethyl]ethylamino]-, dihydrochloride (7CI, 8CI) (CA INDEX NAME)

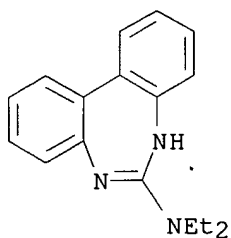


● 2 HCl

10/019,683

RN 2880-34-4 CAPLUS

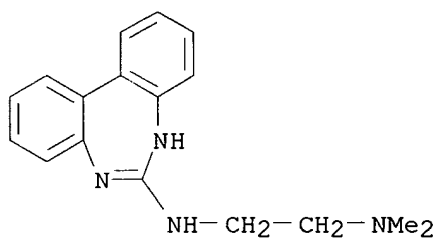
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(diethylamino)-, monohydrochloride (8CI)
(CA INDEX NAME)



● HCl

RN 2880-35-5 CAPLUS

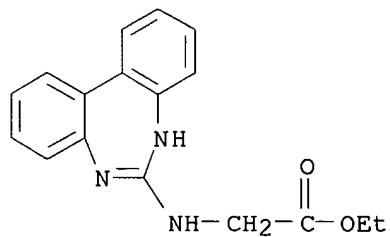
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(dimethylamino)ethyl]amino]-, dihydrochloride (7CI, 8CI) (CA INDEX NAME)



●2 HCl

RN 2880-36-6 CAPLUS

CN Glycine, N-5H-dibenzo[d,f][1,3]diazepin-6-yl-, ethyl ester, hydrochloride (7CI) (CA INDEX NAME)

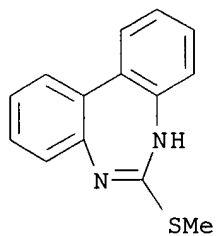


● HCl

RN 2882-40-8 CAPLUS

10/019,683

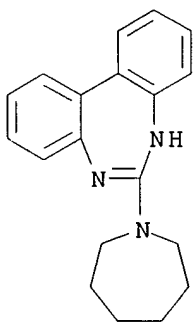
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(methylthio)-, monohydriodide (8CI) (CA INDEX NAME)



● HI

RN 3048-94-0 CAPLUS

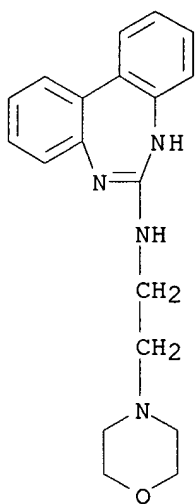
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(hexahydro-1H-azepin-1-yl)- (7CI, 8CI)
(CA INDEX NAME)



RN 3048-97-3 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-[(2-morpholinoethyl)amino]-, dihydrochloride (8CI) (CA INDEX NAME)

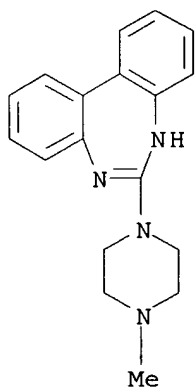
10/019,683



● 2 HCl

RN 3048-98-4 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(4-methyl-1-piperazinyl)-,
dihydrochloride (7CI, 8CI) (CA INDEX NAME)



● 2 HCl

174 ANSWER 55 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1964:404231 CAPLUS

DOCUMENT NUMBER: 61:4231

ORIGINAL REFERENCE NO.: 61:662g-h

TITLE: 6-Amino derivatives of 5H-dibenzo[d,f] [1,3] diazepine

AUTHOR(S): Kreighbaum, W. E.; Scarborough, H. C.

CORPORATE SOURCE: Mead Johnson Res. Center, Evansville, IN

SOURCE: Journal of Medicinal Chemistry (1964), 7(3), 310-12

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

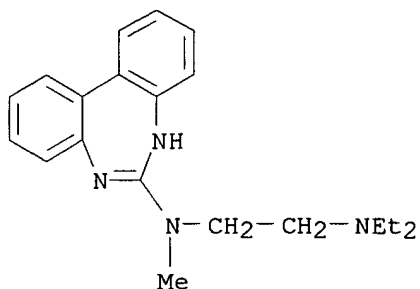
AB 6-Amino and 6-substituted-amino derivs. (I) of 5H-dibenzo[d,f]-[1,3]diazepine have been prepared by replacement of the corresponding alkylthio function or by ring closure of 2,2'-diaminobiphenyl with N,N'-dialkylcarbodiimides or S-methylthiourea.

IT 2849-00-5, 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(diethylamino)ethyl]methylamino]-, dihydrochloride 2849-01-6, 5H-Dibenzo[d,f][1,3]diazepine, 6-piperidino- 2849-04-9, 5H-Dibenzo[d,f][1,3]diazepine, 6-(dimethylamino)-, hydrochloride 2849-05-0, 5H-Dibenzo[d,f][1,3]diazepine, 6-(methylamino)- 2849-06-1, 5H-Dibenzo[d,f][1,3]diazepine, 6-(ethylamino)- 2849-07-2, 5H-Dibenzo[d,f][1,3]diazepine, 6-morpholino-, hydrochloride 2849-08-3, 5H-Dibenzo[d,f][1,3]diazepine, 6-(1-pyrrolidinyl)-, hydrochloride 2849-09-4, 5H-Dibenzo[d,f][1,3]diazepine, 6-(2-thiazolylamino)- 2849-32-3, 5H-Dibenzo[d,f][1,3]diazepine, 6-(butylamino)-, hydrochloride 2849-35-6, 5H-Dibenzo[d,f][1,3]diazepine, 6-(hydroxyamino)-, hydrochloride 2880-29-7, 5H-Dibenzo[d,f][1,3]diazepine, 6-(methylthio)- 2880-30-0, 5H-Dibenzo[d,f][1,3]diazepine, 6-(isopropylamino)- 2880-31-1, 5H-Dibenzo[d,f][1,3]diazepine, 6-(cyclohexylamino)- 2880-32-2, 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(dimethylamino)ethyl]methylamino]-, dihydrochloride 2880-33-3, 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(diethylamino)ethyl]ethylamino]-, dihydrochloride 2880-34-4, 5H-Dibenzo[d,f][1,3]diazepine, 6-(diethylamino)-, hydrochloride 2880-36-6, Glycine, N-5H-dibenzo[d,f][1,3]diazepin-6-yl-, ethyl ester, hydrochloride 2882-40-8, 5H-Dibenzo[d,f][1,3]diazepine, 6-(methylthio)-, hydriodide 3048-97-3, 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(morpholinoethyl)amino]-, dihydrochloride 3048-98-4, 5H-Dibenzo[d,f][1,3]diazepine, 6-(4-methyl-1-piperazinyl)-, dihydrochloride (preparation of)

RN 2849-00-5 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(diethylamino)ethyl]methylamino]-, dihydrochloride (7CI, 8CI) (CA INDEX NAME)

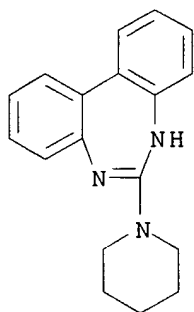
10/019,683



● 2 HCl

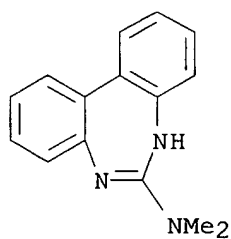
RN 2849-01-6 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(1-piperidiny)- (9CI) (CA INDEX NAME)



RN 2849-04-9 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(dimethylamino)-, monohydrochloride (8CI)
(CA INDEX NAME)

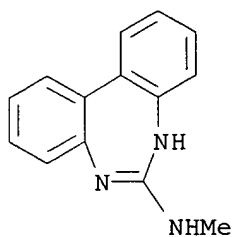


● HCl

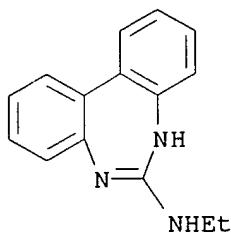
RN 2849-05-0 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepin-6-amine, N-methyl- (9CI) (CA INDEX NAME)

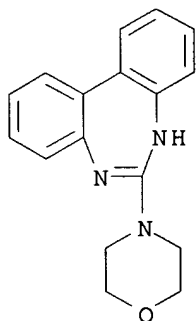
10/019,683



RN 2849-06-1 CAPLUS
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(ethylamino)- (7CI, 8CI) (CA INDEX NAME)



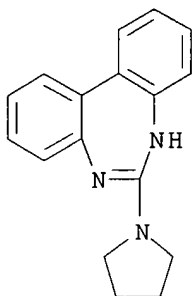
RN 2849-07-2 CAPLUS
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-morpholino-, monohydrochloride (8CI) (CA INDEX NAME)



● HCl

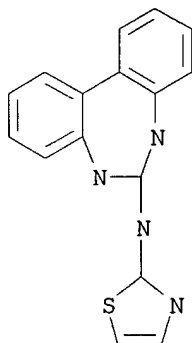
RN 2849-08-3 CAPLUS
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(1-pyrrolidinyl)-, monohydrochloride (8CI) (CA INDEX NAME)

10/019,683

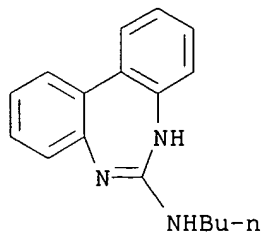


● HCl

RN 2849-09-4 CAPLUS
CN 5H-Dibenzo[d,f][1,3]diazepin-6-amine, N-(2-thiazolyl)- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 2849-32-3 CAPLUS
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(butylamino)-, monohydrochloride (8CI) (CA INDEX NAME)

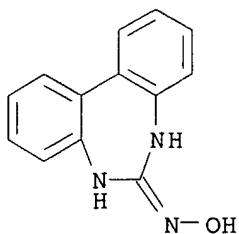


● HCl

RN 2849-35-6 CAPLUS

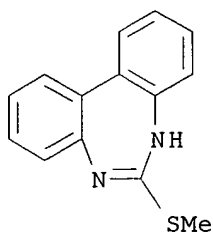
10/019,683

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(hydroxyamino)-, monohydrochloride (8CI)
(CA INDEX NAME)

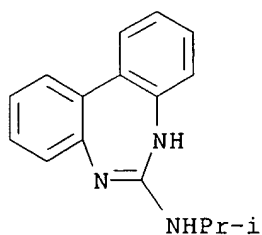


● HCl

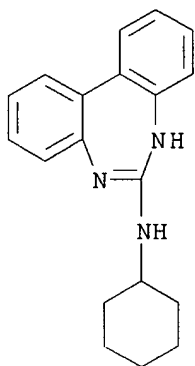
RN 2880-29-7 CAPLUS
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(methylthio)- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 2880-30-0 CAPLUS
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(isopropylamino)- (7CI, 8CI) (CA INDEX NAME)

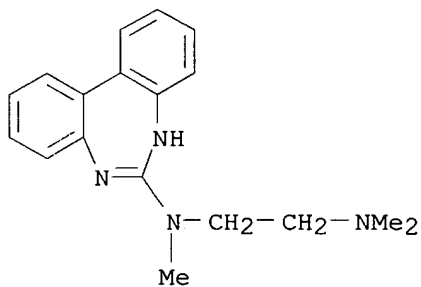


RN 2880-31-1 CAPLUS
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(cyclohexylamino)- (7CI, 8CI) (CA INDEX NAME)



RN 2880-32-2 CAPLUS

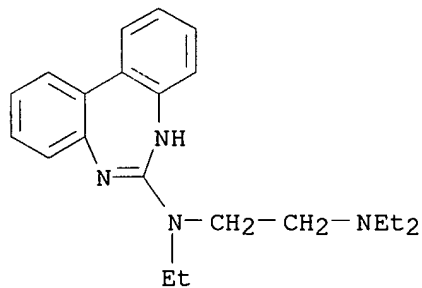
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(dimethylamino)ethyl]methylamino]-, dihydrochloride (7CI, 8CI) (CA INDEX NAME)



● 2 HCl

RN 2880-33-3 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-[[2-(diethylamino)ethyl]ethylamino]-, dihydrochloride (7CI, 8CI) (CA INDEX NAME)

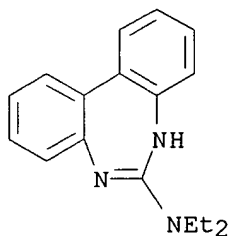


● 2 HCl

10/019,683

RN 2880-34-4 CAPLUS

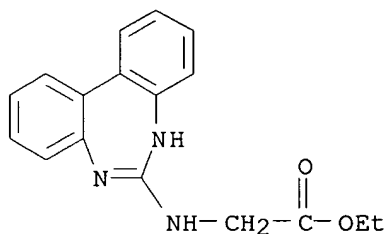
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(diethylamino)-, monohydrochloride (8CI)
(CA INDEX NAME)



● HCl

RN 2880-36-6 CAPLUS

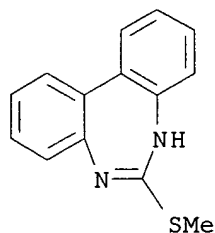
CN Glycine, N-5H-dibenzo[d,f][1,3]diazepin-6-yl-, ethyl ester, hydrochloride
(7CI) (CA INDEX NAME)



● HCl

RN 2882-40-8 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(methylthio)-, monohydriodide (8CI) (CA
INDEX NAME)

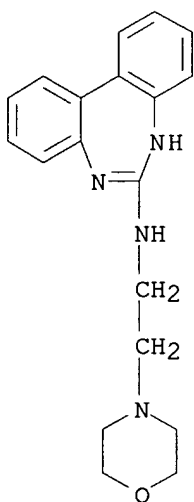


● HI

RN 3048-97-3 CAPLUS

10/019,683

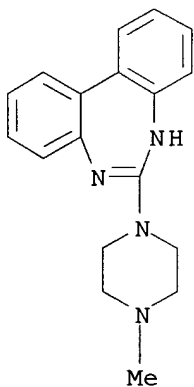
CN 5H-Dibenzo[d,f][1,3]diazepine, 6-[(2-morpholinoethyl)amino]-,
dihydrochloride (8CI) (CA INDEX NAME)



● 2 HCl

RN 3048-98-4 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-(4-methyl-1-piperazinyl)-,
dihydrochloride (7CI, 8CI) (CA INDEX NAME)



● 2 HCl

ANSWER 56 OF 56 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1962:73508 CAPLUS

DOCUMENT NUMBER: 56:73508

ORIGINAL REFERENCE NO.: 56:14297e-i,14298a-i,14299a-c

TITLE: Heterocyclic seven-membered ring systems. XI. Ring closure reactions with o,o'-diaminobiphenyl

AUTHOR(S): Ried, Walter; Storbeck, Werner

CORPORATE SOURCE: Univ. Frankfurt, Germany

SOURCE: Chemische Berichte (1962), 95, 459-72

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 56:73508

GI For diagram(s), see printed CA Issue.

AB cf. CA 54, 5687i. The reaction of (o-H₂NC₆H₄)₂ (I) with carboxylic acids, AcCH₂CO₂Et (II), and ortho esters, and the thermal condensation of mono-Ac derivs. of I are described. I (1.85 g.) and 5 cc. 80% DL-lactic acid heated 5 hrs. on the steam bath, heated slowly during 6 hrs. to 130° pot temperature, cooled, and diluted with 30 cc. H₂O yielded 1.4 g. [o-MeCH(OH)CONHC₆H₄]₂, m. 218.5° (EtOAc). I (9.25 g.) treated with 6.50 g. (CO₂H)₂.2H₂O in 5 cc. hot H₂O, heated 30 min. at 100°, washed with 150 cc. H₂O, and boiled twice with 100-cc. portions MeOH gave 6.0 g. 6,7-dioxo-5,6,7,8-tetrahydrodibenzo[e,g] [1.4]diazocin, m. 186° (decomposition); a similar run with 10 g. (CO₂H)₂.2H₂O gave 9.2 g. product. I (1.85 g.) in 20 cc. o-C₆H₄Cl₂ treated with 1.85 g. o-sulfobenzoic acid anhydride in 15 cc. o-C₆H₄Cl₂, heated 1 hr. at 220° and filtered gave 3.7 g. 6-(o-sulfophenyl)-5H-dibenzo[d,f] [1.3]diazepine, yellow prisms, m. 399° (MeOH). I (1.85 g.), 1.30 g. II, and 5 cc. C₆H₆ refluxed 5 hrs. and evaporated, the residue heated 10 hrs. at 180-200°, and the residual resin (2.6 g.) treated with hot MeOH and filtered gave 0.88 g. insol. 6-oxo-6,7-dihydro-dibenzo[d,f] [1.3]diazepine (III), needles, m. 311-13° with sublimation (AcOH). I (5.55 g.) in 30 cc. C₅H₅N refluxed 24 hrs. with 3.90 g. II and 10 drops piperidine on the steam bath and evaporated, the residue treated with two 50-cc. portions Et₂O, and the insol. material (1.0 g.) recrystd. from AcOH gave 0.3 g. III; the Et₂O solution gave after 48 hrs. 0.08 g. impure III; the Et₂O. solution washed, dried, and evaporated, the resinous residue treated with 100 cc. Et₂O, and the insol. material treated with cold H₂O gave 0.45 g. N-AcCH₂CO derivative of I, m. 93° (decomposition). o-O₂NC₆H₄C₆H₄NHCHO-o (9.7 g.), m. 132°, in 300 cc. 96% EtOH treated with 11 g. amalgamated Al rings, refluxed. 7 hrs. on the steam bath while being treated after 0.5 and 4 hrs. with 6-cc. portions H₂O, kept overnight, diluted with 200 cc. MeOH, heated to 70°, and filtered, and the filtrate evaporated gave 5.8 g. resinous N-CHO derivative

(IV) of I. IV (1.07 g.), 0.75 g. tartaric acid, and 1 cc. H₂O heated briefly gave 1.45 g. hydrogen tartrate of IV, yellow needles, m. 125° (MeOH). o-O₂N C₆H₄C₆H₄NHAc (10.25 g.), m. 160°, reduced in the same manner yielded 8.5 g. pale yellow, resinous N-Ac derivative (V) of I. V (0.23 g.) and 0.23 g. picric acid refluxed in 25 cc. dry C₆H₆ and kept 48 hrs. gave 0.35 g. picrate, m. 239°. Resinous o-O₂NC₆H₄C₆H₄NHCOEt-o (10.8 g.) reduced in the usual manner gave 9.2 g. resinous o-H₂NC₆H₄C₆H₄NHCOEt; a 0.24-g. portion in 5 cc. dry C₆H₆ refluxed with 0.23 g. picric acid in 5 cc. dry C₆H₆, diluted with 10 cc. dry C₆H₆, heated again to boiling, and filtered after 24 hrs. gave 0.2 g. picrate, m. 227-9° (decomposition). IV (7.8 g.) heated 24 hrs. at 225°, cooled, and powdered, and the crude product (2.2 g.) heated with 20 cc. and washed with 10 cc. MeOH gave 1.0 g. insol. material, the filtrate and

washing evaporated gave 0.6 g. yellow resinous 5H-dibenzo[d,f][1.3]diazepine (VI). VI (0.2 g.) and 0.23 g. picric acid in 2 cc. EtOH gave 0.2 g. picrate, m. 233° (MeOH). VI (0.45 g.) in 6 cc. absolute EtOH treated with 0.38 g. tartaric acid in 3.5 cc. absolute EtOH, kept 24 hrs., and filtered yielded the tartrate of VI, pale yellow microcrystals, m. 175° (decomposition) (MeOH), m. 185° (dried 48 hrs. at 50°/12 mm. over P2O5). The MeOH-insol. material (1 g.) dissolved in 120 cc. dry C6H6 and filtered through Al2O3, and the filtrate evaporated gave 0.40 g. VII (R = H) (VIII), yellow needles, m. 282-4°. A similar run with 25g. IV gave similarly 2.6 g. VIII. V (8.5 g.) heated 26 hrs. at 225° yielded in the usual manner 2.05 g. VII (R = Me), yellow needles, m. 285-7°. (o-HCONHC6H4)2 (1.2 g.), m. 137°, heated 0.5 hr. at 260-80°, dissolved in 3 cc. 96% EtOH, and filtered, and the residue washed and dried gave 0.05 g. VIII, yellow needles, m. 270°. VIII (0.388 g.) refluxed 11 hrs. with 15 cc. 96% EtOH and 15 cc. concentrated HCl, filtered, and evaporated, and the residue dissolved in 5 cc. H2O, filtered, and treated with 0.5 cc. concentrated NH4OH gave 0.28 g. I, m. 79°; oxalate decomposed 148°. VIII (0.194 g.), 50 cc. AcOH, and 10 cc. C6H6 reftuxed, cooled, and treated at 24hr. intervals with 1-g. portions solid NaNO2, filtered, and concentrated to 5 cc. deposited 0.12 g. dinitroso derivative dihydrate, m. 134°, which refluxed 32 hrs. with NaOEt-EtOH gave a yellow, infusible Na derivative; no reaction occurred when heated 32 hrs. in HC(OEt)3 (X). The thermal condensation of N-EtCO derivative (11 g.) of I gave 2.9 g. crude VII (R = Et), which filtered through Al2O3 yielded because of strong adsorption only 4 mg. light yellow crystals, m. 276°. I (1.85 g.) and 8 mole equivs. X heated 48 hrs. at 160°, filtered from a high-melting by-product (XI), and evaporated, and the residue dissolved in 12 cc. absolute EtOH with warming and cooled gave 92.7% resinous 6,7-dihydro-6-ethoxy-5H-dibenzo[d,f][1.3]diazepine (XII); the filtrate heated repeatedly to boiling with 2.3 g. picric acid in 12 cc. absolute EtOH gave the picrate of 5H-dibenzo[d,f][1.3]diazepine (XIII), m. 235° (MeOH); XIII.HCl decomposed at 250°; XIII.H3PO4 m. 247° (40% MeOH); XIII hydrogen tartrate m. 186°. A series of runs was prepared in a similar manner (mole ratio X:I, temperature, reaction time in hrs., and % yield of XII given): 8:1, 160°, 24, 82.7; 4:1, 160°, 12, 73.6; 4:1, 20°, 144, 11.8. I and 4 mole equivs. MeC(OEt)3 (XIV) heated 12 hrs. at 150°, evaporated at 190°/17 mm., dissolved in 10 cc. hot C6H6, filtered, and cooled gave 33.6% 6-Me derivative (XV) of XIII, needles, m. 168° (C6H6); XV.H3PO4 m. 285° (decomposition). A similar run during 24 hrs. yielded 24.0% XV and during 144 hrs. at 120° 81.7% XV. I and 2 mole equivs. XIV heated 12 hrs. at 150° gave 51.0% XV. I (0.01 mole) and 0.011 mole XIV in 20 cc. C6H6 heated 12 hrs. at 120° and treated with 1 drop concentrated HCl gave 1.35 g. XV; without HCl in 2 cc. C6H6 at 140° 1.8 g. XV was obtained. XV.HCl was hygroscopic and melted between 80 and 229° (decomposition), depending on the H2O content. XV (4 g.) in 50 cc. 96% EtOH treated with 2.6 g. 85% H3PO4 in 10 cc. 96% EtOH yielded 5.3 g. I.H3PO4, pale yellow platelets, m. 285° (decomposition) (50% aqueous MeOH). EtC(OEt)3 (XVI) (4 equivs.) and I heated 24 hrs. at 180° yielded 24.7% 6-Et derivative (XVII) of XIII, pale yellow needles, m. 232° (C6H6). A similar run at 160° yielded 22.5% XVII. XVII (0.1 g.) in 60 cc. dry Et2O treated with HCl-Et2O gave 0.095 g. XVII.-HCl, m. 204-6°. C(OEt)4 and 0.25 mole equivalent I heated 12 hrs. at 160° gave in 2 identical runs 18.9 and 21.0%, resp., 6-EtO derivative, needles, m. 135° (EtOH); a 0.1-g. portion in 30 cc. dry. Et2O treated with 0.3 cc. concentrated HCl gave the HCl salt, m. 329°; after

drying 48 hrs. at 50°/12 mm., m. 325°. PhC(OEt)₃ and 0.25 mole equivalent I heated 24 hrs. at 160° and evaporated, and the distillation residue crystallized from 15 cc. C₆H₆ gave 58.1% 6-Ph derivative (XVIII) of XIII,

needles, m. 167° (C₆H₆); XVIII (0.1 g.) in 30 cc. dry Et₂O gave 0.11 g. XVIII.HCl, m. 338°. A series of similar runs was performed with a mole ratio of ester to I of 4:1 (reaction temperature, reaction time, and

% yield of XVIII given): 220°, 18 hrs., 46.3; 220°, 12 hrs., 48.1; 20°, 37 days, 85.1. I(5.55g.) and 19.5 cc. X refluxed 24 hrs. at 140°, filtered from some XII, and evaporated, and the residue (4.9 g.) refluxed with 200 cc. absolute EtOH and filtered gave 3.7 g. XII which dissolved in 25 cc. C₆H₆ and diluted with 100 cc. hexane gave 1.3 g. pure XII, m. 164°. XII (0.72 g.) in 3.2 cc. X refluxed 8 hrs. at 160°, filtered, and distilled, and the distillation residue dissolved in 5 cc. absolute EtOH, treated with 0.69 g. picric acid in 7 cc. absolute EtOH, heated

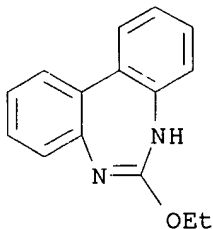
2 min., and cooled gave 0.80 g. picrate of XIII, m. 235°. XI (0.388 g.), m. 303°, treated 11 hrs. at 350° with HCl gave 0.25 g. I. XI (0.4 g.) recrystd. from 50 cc. C₅H₅N gave after 1 month 0.1 g. pure material. The infrared absorption spectra of IX and XV are recorded.

IT 98283-87-5, 5H-Dibenzo[d,f][1,3]diazepine, 6-ethoxy-, hydrochloride 98283-88-6, 5H-Dibenzo[d,f][1,3]diazepine, 6-ethoxy-

(preparation of)

RN 98283-87-5 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-ethoxy-, hydrochloride (7CI) (CA INDEX NAME)



● HCl

RN 98283-88-6 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 6-ethoxy- (7CI) (CA INDEX NAME)

